Structure, dynamics and functions of complex systems*

There were talks introducing the basic ideas, quickly leading up to recent developments in classical chaos (V. Balakrishnan, IIT, Madras); Protein-folding (P. Balaram, IISc.); Self-organized interface depinning (M. Barma, TIFR); Origin of life and biomolecular self-assemblies (M. Vijayan, IISc.); Computers and intelligence (M. Vidyasagar, Centre for Artificial Intelligence and Robotics), and Self-organization and diversity in societies (S. Jain, IISc.). In his inaugural talk, R. Narasimha (IISc. and JNCASR) presented some very recent experimental findings on the effect of volume (ohmic) heating on entrained fluid-flow, suggesting that the prevailing picture of turbulent mixing through progressive *nibbling* at the edges of the boundary layer may have to be replaced by a new one involving a combination of ordered motion, advective chaos and molecular transport. Also, numerical simulation of the flow due to volume-heating shows an enhancement of the short-wavelength spectral weight by several orders of magnitude due to the volume-heating. This calls for a deeper analysis, he said.

There were also presentations covering a wide range of complex phenomena – including neural network model for the kindling of focal epilepsy (C. Dasgupta, IISc.); Dynamical invariants of brain-activities (N. Pradhan, NIMHANS); Circadian clocks (M. K. Chandrasekharan, JNCASR); Genetic-algorithmic study of gene regulation, adaptation, evolution (N. Behera, IISc.); Flash learning (B. Joseph, Cochin University of Science and Technology); Dynamical response of SOC models and earthquake prediction (B. K. Chakrabarti, Saha Institute of Nuclear Physics); SOC in a digging myopic ant model (P. M. Gade, JNCASR); Dynamics of driven diffusive systems with quenched disorder (G. Tripathi, TIFR); Fluid membranes driving and driven by mobile pumps (S. Ramaswamy, IISc.); Spatio-temporal chaos in 2D Fitz Hugh–Nagumo equation (R. Pandit, IISc.); Structure function of Burger and KPZ equation (M. K. Verma, IIT, Kanpur); Fractals and fractions (K. N. Srivastava, Central University of Hyderabad); Solitary waves in liquid crystals (G. S. Ranganath, RRI); Structural transformation in monolayers (K. A. Suresh); Modelling biochemical pathways (S. Sinha, CCMB); Parametric correlations in quantum chaos (Pragya Shukla, JNCASR); Squeezed biophotons (S. Kumar, North-Eastern Hill University) and Population dynamics for two-prey one-predator model (S. K. Srivastava, NEHU).

Deterministic chaos has become a paradigm for complexity of being and becoming. In his comprehensive overview, V. Balakrishnan posed and answered the basic questions that arise with regard to complex systems. How do relatively simple laws lead to richly intricate structures? Why are such structures ubiquitous in the physical world? And how do such complex structures embody their own simple laws of organization? Much interest is now focused on nonlinear, spatially extended, driven, noisy systems. These systems (complex adaptive systems) display very interesting features such as spatio-temporal chaos, pattern formation, edge-of-chaos complexity and self-organized criticality. A specific aspect of complexity is the complex dynamical behaviour associated with deterministic chaos in both conservative and dissipative systems. The role of hyperbolic points in producing chaotic behaviour (exponential sensitivity to initial conditions, loss of information, etc.) was highlighted, with specific examples such as the homoclinic tangle in Hamiltonian systems and dense sets of unstable periodic orbits in discrete time maps. Measures of chaos such as Lyapunov exponents and the Kolmogorov–Sinai entropy were described. The need for a statistical description of chaotic dynamics was brought out, and the role of the invariant density in mixing systems emphasized. Symbolic dynamics and the related concepts of generating partitions, Markov partitions, etc. were discussed in relation to powerful statistical approaches to the analysis of complex dynamical behaviour. Some open problems including the determination of the time-dependent distribution function in chaotic dynamics, and the possible extension of the foregoing to quantum mechanical systems, were also mentioned.

As expected, the protein-folding problem attracted considerable attention. Balaram explained that the problem posed is two-fold – first, how the protein folds so true (the correctness of it) and second, how it folds so fast (the speed of it). The first involves determining the tertiary conformation (the native state) given the primary structure, namely the amino acid sequence forming the long polypeptide chain, known in many cases much in advance from the exhaustive genomic databases. It involves cracking the stereo-chemical code – possibly a second genetic code! The second problem is one of kinetics of relaxation to the global free-energy minimum (or a small set of *taxonomic* minima nearly degenerate). Exhaustive random search would take astronomical time, while actually the natural proteins fold in seconds! This is the Levinthal paradox, now known to be almost irrelevant in that protein folding involves an algorithmic search which is biased kinetically, guided plausibly by topological invariants, and almost certainly informed by the evolutionary entrainment of favourable sequencing. A highly plausible mechanism envisages a moderately frustrating descent into an entropy-enthalpy funnel – a hierarchical free energy-versus-configuration landscape which is, of course, rough with misleading local minima. Initial descent dominated by entropy involves a hydrophobic collapse into a molten globule which is relatively fast. Well defined secondary structures (α-helices and β-sheets) are favoured and retained as correct intermediates that facilitate fast folding. It was pointed out that the recently discovered case of the prion protein (implicated in the mad-cow disease) emphasizes the difficulties of structure prediction and computer simulation of the folding process.

Complexity of self-organization in biological systems is a result of long

*A report of the Discussion Meetings on structure, dynamics and functions of complex systems organized jointly by Jawaharlal Nehru Centre for Advanced Scientific Research and the Indian Complex Systems Society at Bangalore during 10–12 June 1997.

acting evolution. Vijayan dealt with self-organization at two well-separated levels of biomolecular interactions and aggregation, one involving the molecular alphabets of life such as amino acids and the other concerned with large multimeric proteins. Using results obtained in his laboratory on crystalline complexes involving amino acids and peptides, he showed that intrinsic interaction and aggregation propensities could have played a major role in chemical evolution and origin of life, with particular reference to prebiotic polymerization, chiral discrimination and the emergence of the first multimolecular systems. He illustrated the symmetry principle in the quaternary association of subunits in multimeric proteins. Based on the results of the protein crystallographic investigations of his group, Vijayan demonstrated how the symmetry principle can sometimes be violated. Furthermore, there could be interesting situations where small alterations in essentially the same tertiary structure could lead to large changes in quaternary association.

Self-organized criticality (SOC) is a paradigmatic mechanism for generating critical, or scale invariant, complex structures in space (e.g., fractals) and in time (e.g., $1/f$ noise) without fine tuning. Canonical example being a sandpile, though approximate. In some cases, however, the spatio-temporal structure defies visualization as the structure is stationary only with respect to a reference (origin) that itself jumps around erratically over large distances, necessitating a frame co-moving with the centre of activity so as to fix the correlated structure. Mustansir Barma considered one such model, the Sneppen model, for the interface at the depinning threshold on a 2D-lattice of randomly strengthed bonds (quenched disorder) as a result of extremal dynamics (i.e. invading the globally weakest bond) but conserving the interface length. An important result obtained was that the extremal dynamics generated an interface rougher than that for a random-walk model. This sort of structure arises in an entire class of models including the Bak–Sneppen model of biological evolution and diversity. Later, yet another model giving SOC was discussed by Prashant Gade that differed qualitatively from the usual cascade models in that the rough landscape was generated by a single random walker digging according to a set of local rules.

Bikas Chakrabarti introduced an interesting, and potentially important, idea of estimating the distance to a critical breakdown from the measured and calculable dynamic breakdown susceptibilities and critical slowing down for a self-organized criticality. Earthquake prediction was contemplated.

Evolution of and self-organization in a society of interacting selfish agents, following individual mix of available pure strategies, updated constantly on the basis of pay-offs received from other agents, is a problem of great complexity and relevance to population biology and game theory. Sanjay Jain considered a multi-population variant of the governing replicator equation and discussed its attractors. An attractive feature was the emergence of specialization and diversity stable for sufficiently large population of agents in the society.

The question whether or not a given computer can be pronounced intelligent is usually posed and answered operationally in terms of the universal Turing Test, or various generalizations thereof. This was shown to be inadequate for most purposes, and much too anthropocentric. It was proposed that a proper test of computer intelligence should be a test of its capacity to generalize on the basis of learning, or training, on a limited dataset, or set of particular examples – e.g. a multiplication table. Perfect learning is impossible and one must accept the notion of being probably, approximately correct which is operationally quite meaningful.

Neural network model of the brain, with a large number of interconnected 2-state neurons (high/low levels of firing), updated asynchronously by testing for local threshold conditions (potentials), endowed with a Hebbian learning rule (plasticity of synaptic connections) and memory by attractors, captures many features of brain functioning. An insightful phenomenon here is the abnormal kindling of focal epilepsy – generating epileptic seizures in animals (but not in humans!) by repeated electrical or chemical stimulation. Chandan Dasgupta showed through simulation of a simple but biologically relevant model that kindling is due to the formation of a large number of excitatory synaptic connections through a Hebbian learning rule leading to sustained and synchronous firing of the large number of neurons so involved. Its relevance to the nature of memory storage was discussed.

Brain activity is well known to generate tell-tale electrical signals (EEG). N. Pradhan presented a detailed analysis of a multi-channel EEG record by analysing the sampled and digitized time-series for a possible chaotic dynamics underlying the brain activity. Measured correlation dimensions and Lyapunov exponents could be correlated with various brain states like eyes-open, eyes-closed, deep sleep and seizure. Neurobiological significance of these correlates was discussed. Inadequacy of linear stochastic models was convincingly pointed out.

There was a memorable evening lecture by N. Mukunda (IISc) on Existence and Reality in Mathematics and Natural Sciences, aptly complementing and befitting the theme of the Discussion Meeting. With his characteristic clarity and precision, Mukunda presented a scholarly analysis of the deep question of the unreasonable effectiveness of mathematics in the physical universe. It was argued that the Kantian *a priori* synthetic status of mathematics can be re-interpreted consistently with the realization that 'What is *a priori* for an individual is *a posteriori* for the species'. He also advocated the thesis that in the domain of the unknown, far too removed from the 'world of middle dimensions', mathematics may well be the only guide available – hence its evolutionary *raison d'etre!* Its evolutionary advantage is, however, yet to be fully comprehended.

In his opening remarks, K. P. Sinha claimed that the problem of consciousness, like that of the origin of the universe, is one whose time has come. It is a valid object of enquiry that researchers in complex systems must not fight shy of. One could almost sense here A. B. Pippard's well-known lament, 'The invincible ignorance of physics'. He went on to boldly propose an astonishing hypothesis that a new degree of freedom may have to be introduced whose ordering in a complex environment (the neuronal brain) leads to the emergence of consciousness.

In his closing remarks, N. Kumar stressed that the measure of complexity relevant to a highly evolved system is its logical depth which, unlike algorithmic complexity, is low both in the limit of high order as well as high disorder, and peaks somewhere in between – much like some strangeness of proportion. He illustrated this with the help of an artificial genomic sequence generated by a simple algorithm, a re-write rule acting on a 4-letter alphabet, the Rudin–Shapiro sequence. He also wondered if the well-known phenomenon of Shape Memory Effect (SME) observed in the Ni–Ti alloy, the Nitinol marmem, where a large-scale plastic deformation (phenotype) gets encoded into its microstructure (genotype), suggests a kind of allelogenetic regulation – Lamarck's ghost!

The discussion meeting concluded with holding a general-body meeting of members of the Indian Complex Systems Society.

N. Kumar, Raman Research Institute, Bangalore 560 080, India

Bose condensation and the atom laser

R. Srinivasan

The fundamental constituents of matter have an intrinsic quantum mechanical property called the spin. The elementary particles, proton, neutron and electron each have a spin angular momentum of 1/2 in units of $h/2\pi$, where h is the Planck's constant. An atom consists of a nucleus and some extra-nuclear electrons. The nucleus will have a spin depending on the total number of protons and neutrons in the nucleus. Some of the protons will have a spin pointing in one direction (i.e. +1/2) while others will have a spin pointing in the opposite direction (–1/2). The same holds for neutrons and extra-nuclear electrons. The sum total of the spins of all the particles in an atom will have some value which will be integral or half integral. Since isotopes contain different number of neutrons, but the same number of electrons and protons, the total spin of two different isotopes of the same element can be different.

In a gas, a liquid or a solid, many identical atoms are put together. In a gas the interaction between the atoms is weak as the inter-atomic separation is large. In a non-interacting gas, one may consider the total quantum mechanical state of the gas to be made up of a product of individual one-particle states. The behaviour of the many body quantum mechanical state when two of the indistinguishable atoms are interchanged will depend on the total spin of the atom. If the total spin is zero or an integer multiple of $h/2\pi$, then the many body wave function will not change when two atoms are interchanged. One consequence of this property is that any given single particle quantum state can be occupied by any number of particles in the system. Such a system is described by Bose statistics, first postulated by S. N. Bose. On the other hand if the atom has half integral spin then the many body quantum mechanical wave function will change sign when two atoms are interchanged. In such a case a given quantum mechanical one particle state can only be occupied by zero or one particle in the system. Such a system obeys the Fermi–Dirac statistics. At very high temperatures the two statistics approach in behaviour classical statistics proposed by Boltzmann. However at low temperatures the two different quantum statistics predict different behaviour. In Fermi–Dirac statistics, at absolute zero all quantum states with an energy lower than a certain value E_F are occupied, each by one particle. All states with energy greater than E_F are unoccupied. On the other hand in Bose statistics as the temperature is reduced, more and more particles can get into the one-particle ground state. This becomes an avalanche below a certain temperature T_c called the condensation temperature. Below T_c a macroscopic fraction of the number of particles occupies the ground state and this fraction increases as the temperature is lowered below T_c. This is a phase transition and is accompanied by a change in the specific heat at T_c. This transition is similar to condensation in real space, though the condensation in the Bose gas occurs in phase space consisting of the position coordinates and the momentum components of all the atoms. This distinctive feature of Bose statistics was pointed out by Einstein.

Experimental attempts to see Bose condensation in a gas failed because at the densities prevalent under normal pressure, there is an attractive interaction between molecules of a gas. This attraction is strong enough to cause a vapour-to-liquid-phase transition to occur before the Bose condensation temperature is reached. In a dense liquid in which intermolecular interactions are strong, the theory of Bose condensation between the quasi-particles is considerably modified. The superfluid transition seen in liquid ^4He at 2.17 K is believed to be due to Bose condensation, though no satisfactory quantitative theory has yet been worked out to account for the properties of superfluid ^4He.

To observe Bose condensation in a weakly interacting gas, one uses atomic vapours. In atomic vapours, two conditions are required: namely that (i) the density of the vapours be low (10^{11} to 10^{14} atoms/cc) to reduce considerably the interatomic interactions, and (ii) the vapours be cooled to temperatures below T_c which, at the above mentioned densities, is usually below 1 μK. Obviously such vapours have to be produced in ultra-high vacuum (pressure ≈ 10^{-9} to 10^{-10} mbars). To cool these atoms, one uses lasers. When the atoms are placed in a region in which appropriately tuned counter-propagating laser beams in three orthogonal directions meet, absorption and re-emission of the photons cause the atoms to lose their kinetic energy and to cool to a temperature of the order of 50 μK. Such an arrangement is called the optical molasses. To trap the atoms for a sufficiently long time and to cool them to the above temperature, one uses a magneto-optical trap. In this trap a small mag-