RÉSUMÉ

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Date of Birth	13 April 1966
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Degrees Obtained

1995 **Ph.D** in Theoretical Condensed Matter Physics,
Indian Institute of Science (I.I.Sc), Bangalore, India.
Thesis Title: 'Equilibrium and Nonequilibrium Dynamics of Dense Liquids'.
Thesis Supervisors: **Prof. Sriram Ramaswamy** and **Prof. Chandan Dasgupta.**
(Awarded Junior and Senior Research Fellowships by the Council
for Scientific and Industrial Research (C.S.I.R), Govt.of India.)

1988 **M.Sc** in Physics, University of Poona, Pune, India.
(Tata Institute of Fundamental Research (T.I.F.R) -
University of Poona Joint M.Sc Program).
Specialization: Condensed Matter Physics.
Project: 'Cellular Automata'.

1986 **B.Sc**, St. Joseph's College for Arts and Science, Bangalore, India.
Major Subjects: Physics, Chemistry, Mathematics.

Career Highlights

- October 2001-March 2003: Post Doctoral Fellow at the Modelling, Simulation and Design Lab (MSDL), School of Computer Science, McGill University, Montréal, Canada.
  Research (with Prof. Hans Vangheluwe): Introduction of computer algebra features into AToM^3, a tool for meta-modelling and simulation developed at MSDL.
- May 2000-April 2001: Research Assistant at the School of Computer Science, McGill University, Montréal, Canada.
  Research (with **Prof. Sue Whitesides**): Study of the effect of shape on the surface tension – induced self-alignment of polymer cookies.
- June 1998-November 1999: Research Fellow at the Department of Applied Mathematics, Biometrics and Process Control (BIOMATH), University of Gent (RUG), Gent, Belgium.
  Research (with **Dr. Hans Vangheluwe** and **Prof. Peter Vanrolleghem**): Modelling of activated sludge sedimentation, and symbolic transformation of partial differential equations (PDEs) into differential algebraic equations (DAEs).
- March 1997-February 1998: Consultant to the Year-2000 (Y2K) Solutions Group at Intertec Communications Private Limited (ICPL), Bangalore, India.
  Work: Developed Y2K Testing Strategies, participated in the specification and testing of an in-house tool developed to automate Y2K solutions.
- March 1995-June 1996: Post Doctoral Fellow at the Max Planck Institute for Colloids and Interfaces, (MPI-KG), Berlin, Germany.
  Research (with **Prof. Reinhard Lipowsky**): Study of membranes with anchored polymers at the adsorption transition.

List of Publications

1. *Membranes with anchored polymers at the adsorption transition.*
   C.Hiergeist, A.V. Indrani and R. Lipowsky, **Europhys. Lett. 36 (7)**, 491 (1996).
2. *Shear-induced enhancement of self-diffusion in interacting colloidal suspensions.*
   A.V. Indrani and Sriram Ramaswamy, **Phys. Rev. E**, **52 (6)**, 6492 (1995).
3. Reply to Comment on *Universal self-diffusion and subdiffusion in colloids at freezing.*
   A.V. Indrani and Sriram Ramaswamy, **Phys. Rev. Lett.**, **74 (8)**, 1491 (1995).
4. *Universal self-diffusion and subdiffusion in colloids at freezing.*
   A.V. Indrani and Sriram Ramaswamy, **Phys. Rev. Lett.**, **73 (2)**, 360 (1994).
5. *Is there a growing correlation length near the glass transition ?*
   C. Dasgupta, A.V. Indrani, Sriram Ramaswamy and M.K. Phani,
   Europhys. Lett., **15 (3)**, 307 (1991).

Unpublished Reports

1. *An algorithm to implement a canonical representation of algebraic expressions in AToM^3.*
   Hans Vangheluwe, A.V. Indrani and Bhama Sridharan, MSDL report (2003).
2. *Some issues concerning Computer Algebra in AToM^3.*
   A.V. Indrani, MSDL report (2002).
3. *A comparative study of moments of inertia of some plane figures including polygons, crosses and flowers.*
   A.V. Indrani (2001).
4. *WEST++: Implementation of two test case PDEs using the Orthogonal Collocation method.*
   A.V. Indrani, BIOMATH report (1999).
5. *WEST++: Allowed forms of PDEs and boundary conditions that can be solved using the Orthogonal Collocation method with matrices .*
   A.V. Indrani, BIOMATH report (1999).
6. *WEST++: Transformation of a given PDE to a DAE using the Orthogonal Collocation Method on Finite Elements.*
   A.V. Indrani, BIOMATH report (1999).
7. *Optimal number and types of test cases for various critical and non-critical usages of date variables in Y2K-candidate programs.*
   A.V. Indrani, ICPL Internal Document (1997).

Conferences and Meetings attended

- Attended the *Intensive Course on Modelling and Simulation* given by Dr. Hans Vangheluwe, organized by the Centre for Continuing Education, I.I.Sc, at I.I.Sc (1998).
- Posters presented (by advisor Prof. Ramaswamy) at the *Gordon Conference* on *Complex Fluids*, Germany, titled *'Shear-induced enhancement of self-diffusion in interacting colloidal suspensions'* and *'Universal self-diffusion and subdiffusion in colloidal liquids at freezing'* (1993).
- Poster presented at the Discussion Meeting on *Dynamics of Fluid Phases*, J.N.U, New Delhi, titled *'Shear-induced enhancement of self-diffusion in interacting colloidal suspensions'* (1993).
- Poster presented at the annual *D.A.E. Solid State Physics Symposium*, B.A.R.C, Bombay, titled *'Is there a growing correlation length near the glass transition ?'* (1991).
- International Conference on *Complex Fluids and Polymers*, organized by I.I.Sc and J.N.C.A.S.R, at I.I.Sc (1990).
- Indo-Soviet Meeting on *Phase Transitions and Critical Phenomena*, organized by I.I.Sc and J.N.C.A.S.R, at I.I.Sc (1990).
- Discussion Meeting on *Open Problems in Condensed Matter*, at the Dept. of Physics, I.I.Sc (1989).
- Summer School on *Astronomy and Astrophysics*, at I.I.Sc (1987).

Computational Experience

All the problems addressed in my Ph.D thesis involved extensive numerical work. The computational procedures used are described briefly in the summary of my research work. I have used the Computer Algebra tools MAPLE and MuPAD, and to a small extent, the minimal-surface generation tool Surface Evolver. I have used the modelling and simulation tools WEST++ and AToM^3 to build example PDE and algebraic equation models respectively. As a Consultant to the Y2K Group at ICPL, I developed programs in a Query Language which was part of Vision:Inspect, a COBOL-parser based software engineering tool. These programs greatly enhanced the speed and accuracy of detecting date variables in COBOL programs.

Summary of Research Work

- ***Growing correlation length near the glass transition:***

  This work consists of a numerical analysis of data obtained from a molecular dynamics simulation of a Lennard-Jones binary mixture, in a search for a growing correlation length, and any bond-orientational ordering near the glass transition. In particular we look for evidence of *icosahedral* order. To look for a growing correlation length, the system-size dependence of the relaxation times of bond-orientational correlation functions is studied, and compared to a similar analysis of density correlation functions. Our results are the following:
  (a) there is no particular tendency towards icosahedral ordering near the transition;
  (b) no effects of finite-size can be seen in the orientational relaxation times near the transition;
  (c) orientational and density correlation functions decay in a very similar manner, and we can identify the same temperature for the glass transition using either of them. The growth in relaxation times of both density and orientational correlations is of similar magnitude. Our results for orientational correlations match those for density correlations, and allow us to conclude that there indeed is *no* growing correlation length near the glass transition. This conclusion questions certain earlier theories that claim the existence of an underlying continuous phase transition whenever a liquid forms a glass.

  This problem involved analyzing data from the molecular dynamics simulation of a three dimensional lattice gas model to calculate space and time dependent orientational correlation functions. This was done by defining a suitable discretized orientational order parameter field in terms of spherical harmonics. The programs were written in FORTRAN.

- ***Self-diffusion in colloidal liquids at freezing:***

  In this work we study the suppression of self-diffusion in colloidal liquids at freezing. We provide a theoretical explanation for the observed quasi-universality of D_L/D_0, the ratio of the long-time to short-time self-diffusion coefficients for different colloidal liquids (interacting with different potentials) on the freezing line. This is the 'dynamical freezing criterion' seen in experiments and Brownian dynamics simulations. We also predict that the mean squared displacement at freezing, plotted against a suitably renormalized time, yields a universal curve showing a short-time sub-diffusive regime and a long-time caged diffusion. We obtain the incoherent part of the intermediate scattering function $C_s(k,t)$, for all wavenumbers k and times t, and show that it implies strong non-Gaussian behaviour in the probability distribution of the single particle displacement at short times.

  This problem involved using the pseudo-spectral method to calculate the relevant correlation functions, and subsequently the static structure factor. This mainly consisted of performing numerical Fourier transforms in space and time for a certain kernel iteratively, till self-consistency was achieved. Existing Fast Fourier

Transform (FFT) packages were not flexible enough for this purpose, so my programs performed the Fourier transforms directly using standard numerical integration and interpolation routines. The programs were written in FORTRAN.

- ***Enhancement of self-diffusion in an interacting colloidal liquid in a shear flow:***

  Here we examine some unusual features of the self-diffusion coefficient in an interacting colloidal suspension driven away from equilibrium by a shear flow. In particular, we obtain theoretically the shear-induced enhancement of self-diffusion, which has been observed both in experiments and in simulations. We set up generalized Langevin equations describing coupled single-particle and collective motions in a suspension of interacting colloidal particles undergoing shear. We show that the self-diffusion coefficient should be strongly dependent on shear rate Ω. Three regimes are found: (a) an initial *const.* + Ω^2 followed by (b) a large regime of $\sqrt{\Omega}$ behaviour, crossing over asymptotically to the Stokes-Einstein value D_0 as (c) D_0 - *const.*/ $\sqrt{\Omega}$. We also find that the shear-induced enhancement is *isotropic*, until we reach very large shear rates. This direction-independence of the enhancement is also in agreement with experiments and simulations. Our simple theory explains how shear enhances self-diffusion by a reduction of the effective friction felt by a colloidal particle because of its interactions with other particles.

  This problem involved evaluating a very complicated three dimensional nested integral (seven nested integrals in all) to find the shear-induced self-diffusion coefficient. Existing numerical packages proved inadequate to handle the problem. Therefore I had to develop a new algorithm which used a combination of standard integration routines for the nested integrals, and evaluated the integration over volume as a weighted sum over vertices located within a sphere. This yielded a drastic reduction in computing time. The programs were written in FORTRAN.

- ***Membranes with anchored polymers at the adsorption transition:***

  Polymers which are anchored to membranes exert bending moments onto these soft surfaces. We show that an ideal polymer anchored to a membrane and interacing with it can affect the membrane's elastic properties in interesting ways. We have obtained the renormalization of the elastic moduli of the membrane over the entire regime of the polymer-membrane interaction, between the two extremes when the polymer is entropically repelled from the membrane, and when it is totally adsorbed. A parameter that characterizes this interaction is b, the inverse extrapolation length. b varies over $[-\infty, +\infty]$ as the polymer goes from being strongly adsorbed to being completely desorbed from the membrane, and is exactly zero at the adsorption-desorption transition. Also, a study of the spontaneous curvature of the membrane shows that tuning the polymer-membrane interaction can induce a change in its sign: in the adsorbed regime, the membrane likes to curve towards the polymer, while in the desorbed regime it curves away from it. Another result we obtain is that, over the whole range of b,

the membrane's bending rigidity and Gaussian bending rigidity are renormalized in opposite ways.

The work done here was mainly analytical, and the Computer Algebra tool MAPLE was used in simplifications.

- ***Modelling and simulation of a secondary settler using PDEs:***

  Engineers have employed simplified, 'coarse grained' models of the complex process of sedimentation of activated sludge in a Waste Water Treatment Plant (WWTP), using several one dimensional (1-D) PDEs. We have proposed one such set of PDEs to describe the 'continuous' and 'batch' sedimentation processes in secondary settlers, with corresponding boundary conditions. For this class of 1-D PDEs, their symbolic discretization based on orthogonal collocation over finite elements is implemented within the WEST++ Modelling and Simulation environment developed at BIOMATH, using computer algebra techniques. In particular, a general expansion procedure, eventually suitable for N-D problems of more general nature than the sedimentation PDEs, has been devised and implemented within the WEST++ Model Compiler. The symbolic discretization is automatic and transparent to the user. It allows for a uniform treatment, and global symbolic optimization, of the Ordinary Differential Equations (ODEs) and PDEs occuring in a complete WWTP model. Such a model always contains a high degree of (non-linear) feedback. The symbolic approach leads to more insight, higher performance and numerical stability than purely numerical approaches. A procedure has been constructed to detect linear and non-linear equations and perform the appropriate discretization. In particular, certain non-linearities in the boundary conditions are replaced symbolically by piecewise linear approximations. This leads to higher computational speed and accuracy.

  Examples were implemented within WEST++ using its Modelling and Simulation Language (MSL).

- ***The effect of shape on the surface tension induced self-alignment of polymer cookies:***

  It has been observed in microfluidics experiments that pairs of two-dimensional hydrophilic polymer objects ('cookies') of a given shape align themselves so that the shapes match perfectly, when one cookie is dropped on top of the other with a drop of liquid in between. The liquid wets the cookie surfaces completely, and it is the liquid drop which pulls the cookies into alignment while trying to minimize its surface tension. An interesting question is which shapes are the best ones to achieve this alignment. This theoretical study addresses different shapes used in the experiments, such as polygons, crosses, flowers, in an effort to understand the effect on the alignment of sharp corners and their number. This is done by considering the energy of the cookie-water system for an arbitrary relative orientation of the cookies, and minimizing it to obtain the equilibrium aligned configuration.

  This work was mainly analytical, with some preliminary work done using the minimal-surface generation tool Surface Evolver.

- ***Canonical representation of algebraic expressions in AToM^3:***

  AToM^3 is a multi-paradigm modelling and simulation tool developed at the MSDL lab at McGill University. In order to symbolically manipulate, and therefore solve more efficiently, the differential algebraic equations (DAEs) generated during modelling of complex systems, certain computer algebra features need to be added to AToM^3. Rather than plugging in existing bulky computer algebra systems such as MuPAD, it is preferable to develop in-house, symbolic manipulation features tailored to solve DAEs. As a first step, we have proposed an algorithm for a practical canonical representation to store algebraic expressions and equations internally in AToM^3. Algebraic equations (containing constants and variables) can themselves be modelled graphically in AToM^3, and a canonical transformation that can be invoked from within the tool has also been implemented. This renders the equations in a canonical form.

  An example of symbolically solving a set of DAEs was implemented in MuPAD as a proof of concept. A set of four equations was symbolically analyzed by performing dependency analysis and causality assignment. This was done by finding a maximal flow on a bipartite graph defined over the equation numbers and the unknown variables, using the network algorithms of MuPAD. Further, the equations were sorted (in the order in which they should be solved) using a topological sort program of MuPAD, with a few modifications.