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The Students' Voice of IIT Madras

*presents*

# IMMERSE

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## *From the Editor's Desk.*



*Immerse is IIT Madras' Magazine on Research in Science and Engineering. Our endeavour is not only to showcase some of the recent developments in research and innovation at IIT Madras, but also to communicate the science behind them through articles which can be understood even by those new to the field. We hope that through these articles, the reader gets a flavour of the research happening in various parts of the institute.*

*In this year's issue, we have articles covering a wide range of research areas - ranging from topics like neurodegenerative disorders to understanding the chaotic dynamics of flapping of bird wings and trying to decipher the void between stars in the night sky.*

*We take this opportunity to thank the Director and the Dean of Students for their unflinching support to Team Immerse. We also thank our sponsor, Caterpillar, without whom this edition would not be possible. We would like to express our gratitude to the professors and their research students, for their valuable time and support, throughout the process of making the magazine. Last but not the least, we would like to thank The Fifth Estate and the Shastra sponsorship team for their support.*

*Without further ado, we invite you to immerse yourself in the 6th edition of Immerse.*

Sriraghav, Malayaja, Mythreyi, Ivana, and Praneeth  
Immerse Editorial Team 2017-18

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# Immerse

*IIT Madras Magazine on Research in Science and Engineering*



# E



# CATERPILLAR

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# Future is here: Age of Smart Sites

*Caterpillar Engineering & Technology Center - India*

We have all witnessed iron flexing its muscles in the last decade, from autonomous cars to the autonomous construction machines, we are quite close. But where is it leading us to? For the Construction and Mining industries, next couple of years will be the 'Age of Smart Sites'.

In the next couple of decades, we should not be surprised if we see a building or a road getting constructed without any human intervention and the only humans involved are sitting hundreds of miles away in a corporate air-conditioned office monitoring these machines live as they are creating the future. As we watch, autonomous/driverless cars and machines moving ahead, we should realize that a new dimension in technology spectrum is unfolding in front of us. Few of the areas which are must for a smart site are:



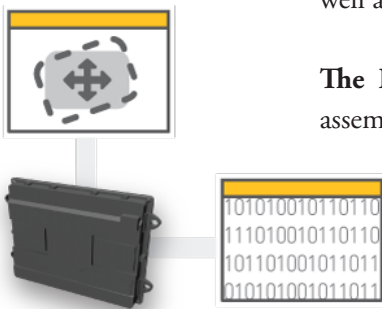
**Eyes of the machine:** All the earlier camera technology from Lidar to Kinematics have taken flight. Now we have cameras available in size of a cricket ball that can be mounted on a truck or a machine or a car providing real time feed to the machines for further analysis and processing. You can easily buy one on Amazon now.



**Sense of the machine:** We have taken off from traditional definition of a sensor as well here, machines these days are equipped with radar based, infra-red sensors. This has enabled the machines to get critical data at a required precision, which was not possible earlier. Now we can collect all the smart sensors information and pass it on to the brain of the machine.



**Machines Nerve Network:** Last 5 years has also seen a step change on a car or machine network. On a car or machine, we need a reliable and robust connectivity at Giga Bit of speed. Industry went through many technologies and currently settling down on two-wire Ethernet but it is needless to say that we are going to soon exhaust GigaBit speed as well and we will need something better. To put it right we will need limitless speed.



**The Brain of the Machine:** A car or a machine these days is divided into many assemblies, usually each assembly has its own controls and ECUs. From one perspective, we differ here how a human work but if you go a little deep you can see machine assemblies as a nuclear family. Each individual of the family bringing its own unique value proposition to ensure success of the family. So, this area is managed in two ways currently :

- a) Increased CPU power
- b) Multiple CPUs to not to hit a limit

**Memory:** With silicon getting cheaper, cost and volume required to store data has gone down drastically in past two to three decades. Without this, it would have not been possible for us to get where we are today.

**Society:** On a site, if machines have to work then they need to communicate with each other and each machine should be able to tell its neighbor on good and bad things going in its life. Essential element for it is machine to machine communication. Various start-ups, alliances and companies are focusing on technology spectrum that will enable machines to communicate with each other. Few of the pioneers are LoRa Alliance, Filament etc. We are pretty close to see this happening at an affordable cost.

**Collective Consciousness:** Sites can run in acres and machines can be distributed in the corners of the site with a close tie on site performance. Now to ensure all are working towards one goal, what we need is a collective consciousness, isn't it how humans work? We need a way through which collectively for the society of the machines a general context and awareness can be set. It has very wide implications as multiple machines on site will be setting up a AI based neural network which should be processing a terabit of data to arrive at "How we are doing collectively?", "What are our common problems?", "When to lay down a helping hand?". As we develop a collective consciousness the question to be asked here is "How do we keep unhealthy competition away?"



**Collective Planning and Execution:** Our society of machines, would have a leader as well who would take the last call. On a mining site, it can be very well a dragline or on a road construction site it can be very well a paver but our society of machines need to participate in a collective planning and commit to targets to arrive at overall plan. It would be in-efficient to do the same at the machine itself, so we may need to create those machines bots/avatars in the cloud who can do effective planning and stay in sync with what's happening on the ground.

As you can see, we are already talking about bots doing negotiation or a neural network for a collective AI or a Lidar camera fitted on a drone. We are close to having our subsystems in place, that's what makes us confident that next two decades will realize the "Age of Smart Sites". With that welcome to the "Welcome to the age of smart iron" and get ready for the "Age of Smart Sites".



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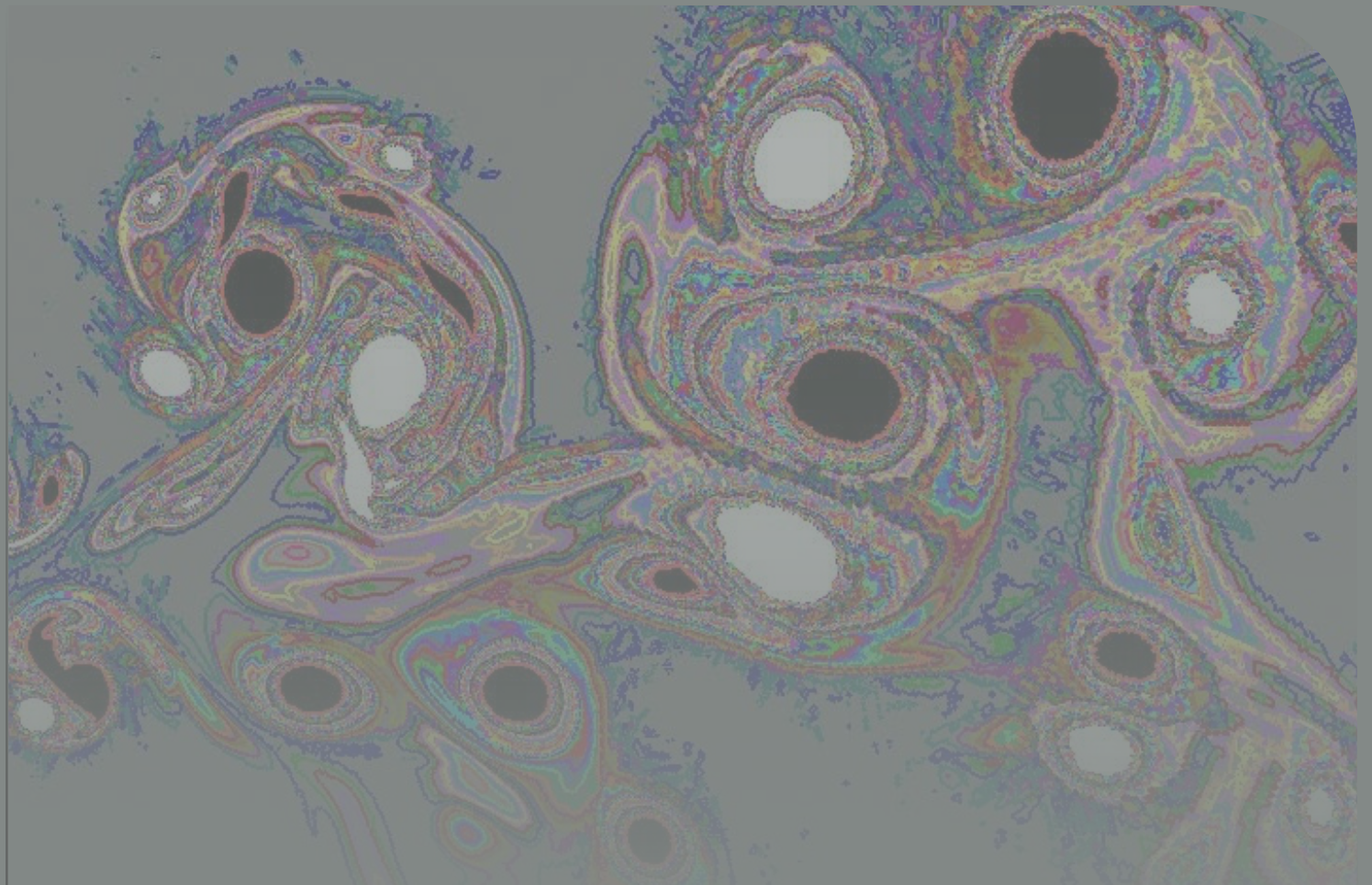
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*What the voids have in store*



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# UP IN A FLURRY

## *The Chaos Behind Natural Flight*

by Shivani Guptasarma

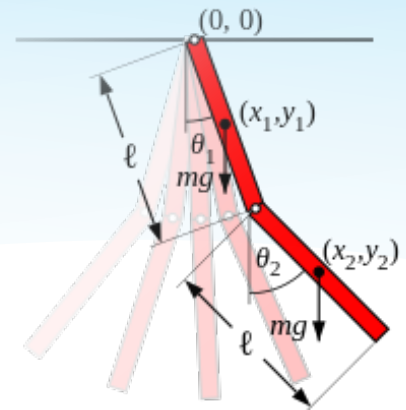
*Human-built air vehicles glide, chop, or propel themselves through the air. Nature's fliers, however, flap their wings. Flapping flight is a complicated phenomenon, and understanding it could help to truly imitate natural flight someday.*



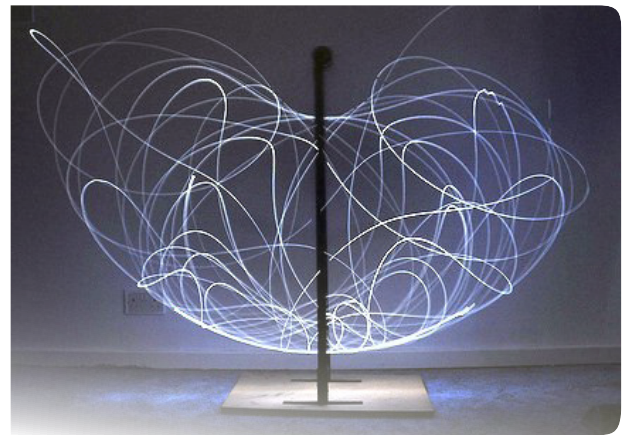




Who would have thought that the pendulum – the staid symbol of predictability and rhythm – could behave so wildly when doubled? The brain searches in vain, thinking it has caught a pattern here, a structure there, when, without warning, everything goes haywire again. Watching a double pendulum swing is in some ways like listening to a piece by Stravinsky, or reading a poem with no meter. Such unpredictable behaviour is not the exception but the norm in nature, Dr. Sunetra Sarkar tells us as we sit in her office late one Friday evening, talking about how birds and insects fly. After centuries of admiring natural flyers and longing to imitate them, there is a reason why only a handful of our flying machines come anywhere close to the dream of flying like a bird, with the flapping of wings and the freedom to perch, hover and take off at will. Natural flight is something that humans have not been able to fully understand despite millennia of effort, even now that we have the equations describing fluid flow at our disposal. Dr. Sarkar and her group at the Department of Aerospace Engineering work at the intersection of fields, combining dynamical systems theory with unsteady aerodynamics to understand these processes.



One might wonder what is unpredictable about classical physical systems on a macroscopic scale with no quantum physical phenomena involved. After all, if the position and velocity of all particles in the system is known at a certain time, Newton's laws dictate the entire future of the system. How the double pendulum is configured when it starts swinging should dictate how it behaves later. How a bird flaps its wings should determine exactly how the air flows around it.

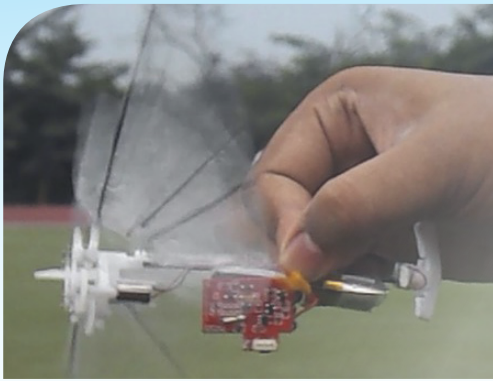


This is perfectly true in principle. Two kinds of mistakes, then, can keep us from seeing why we are unable to predict the behaviour of some systems. First, we take for granted that it is possible to know the starting configuration of a system exactly. This is all very well in mathematics, but never happens in real life. Second, we naïvely imagine that if we know the starting configuration approximately, then we should be able to predict the future behaviour approximately. Our minds somehow assume that the system is linear, that the result of a slightly wrong input would be a slightly wrong output. However, not all systems are linear. In chaotic systems, a tiny change in input can alter the behaviour beyond recognition. The weather is chaotic, hence the phrase “unpredictable as weather” and the Butterfly Effect description of chaos: a butterfly flapping its wings in a rainforest can cause a tornado weeks later halfway across the world. A double pendulum is chaotic as well, and so is the flow of air around a flapping wing, explains Chandan Bose. As a doctoral research scholar studying the dynamics of natural flight with Dr. Sarkar and Dr. Sayan Gupta (at the Department of Applied Mechanics), Chandan works to understand the physics of chaos, and how birds use it to fly. An enthusiastic member of the institute's Aero Club at the Centre For Innovation, he also builds flapping wing prototypes, both to study and for fun. As it turns out, these are entirely different from other flying vehicles, such as planes, and single or multi-rotor helicopters.



*One of the flapping mechanisms built by Chandan*

Blowing air over a strip of paper is a nice demonstration of the principle behind the flight of planes. Since air flows faster above the strip, the air pressure is higher below it than above, and this pushes the paper upward. An aeroplane wing is designed with a shape that forces



*The artificial insect in action*

the air above it to move faster, even when the oncoming stream of air arrives with a uniform speed. The plane first speeds up on the runway to get the air streaming past it to move fast enough. The shape of the wing does the rest by creating pressure difference, so that the craft receives enough lift from the air to overcome its own weight. It is also important that the shape of the plane be streamlined, or else the drag from the air would put up too much resistance to any movement.

Things are different when a bird or an insect flies. It needs neither runway nor landing strip. It could have the clumsiest imaginable shape and still manage to move through the air without any trouble. It knows how to avoid crashing into things on its way, how to stop when it needs to, and how to react to changing winds and to other flying objects. To paraphrase what Leonardo da Vinci said a millennium ago, and what Dr. Sarkar says now, human beings are intelligent and creative, but often the best thing that we can do with these capabilities is to use them to learn from the usually superior designs of nature. The equations governing the way fluids such as air and water move were figured out a couple of centuries ago, as a culmination of contributions from a series of thinkers. Called the Navier-Stokes equations (NSE), they are a set of equations which tie together fundamental physical laws – the conservation of mass, energy and momentum – with the properties of the fluid in question, such as its density and viscosity. They do this in a way that relates the flow of the fluid to the pressures at different places.

Imagine standing somewhere in the middle of a stream, noting how fast the water flows past your feet and in which direction. Theoretically, if this could be done at every point in the stream at once, then the flow at that instant would have been completely described. This is how Euler, the great mathematician, looked at flow – the way a fluid flows is described by treating it as a set of velocities in space, a “velocity field”, which changes with time. Since the velocity field describes a quantity that changes with both time and location, the NSE do not talk about velocity directly. They are partial differential equations instead: they tell us how the velocity at a certain point in the region changes with time, how the velocity at a frozen instant in time changes as one looks at different locations, and so on. These equations must be solved to find the velocity field, before one can see how the fluid actually behaves. Surprisingly, not only do we not have a general solution for the NSE, we do not know how to say for sure whether a solution even exists.

In such situations, there are two avenues available to engineers, and they choose whichever works best. The first is to make assumptions, treating the system as a simpler one than it really is. This reduces the complexity of the equations and sometimes they become open to an analytical solution. This solution is a mathematically perfect fit for the equations in question; the trouble is that the equations themselves may no longer fit the physical system that they are meant to represent.

The second method is to find an approximate solution to the equations. This is done by dividing space into a grid, treating it as a collection of points – many, but not infinitely many. Time, too, is treated not as continuously varying but as a series of steps, a chain of moments. This allows us to find something that is not quite the exact solution, but is close. Say we were trying to guess at an invisible smooth curve on a sheet of paper, given a string of a hundred closely spaced points on it but not the curve itself. One could get a reasonable picture of reality by joining consecutive points with straight lines, or for that matter tiny parabolic segments. Numerical solution techniques generalise this idea. How one chooses to join the points, how many points are necessary to consider the result reasonably close, how close is “reasonably close” – all these depend on the system in question, the judgment of the researcher, and how powerful a computer is available. The finer the grids and the smaller the time step, the closer we get to a realistic idea of the physics, and the more difficult it is to actually compute the solution. Today, it takes Chandan weeks and often months of processing to run a single simulation on the Virgo Super



Cluster at IIT Madras – one of the country’s most powerful supercomputers running his code day and night on 16 processors simultaneously. These are high-fidelity simulations, which means that they are based on a bare minimum of assumptions and therefore work on equations that quite accurately describe the physics of the system. Fifty years ago, Dr. Sarkar remarks, there was no question of solving such equations in any reasonable amount of time without making drastic assumptions to simplify them.

The first reason why the dynamics of flapping are so different from those of a stationary wing is the the effect of time. A stationary wing facing a steady wind has the same flow around it as long as the flow speed does not change, but air around a flapping wing flows past a structure whose position and orientation changes all the time. Then there is layer upon layer of complexity. For one thing, even if one assumes that the wing moves in a repeated pattern over regular intervals, this motion is not a simple up-and-down “plunging”, but is more complicated in reality, involving forward-and-backward tilting as well. To add to this, the wing is a flexible body. It not only flaps in complex ways, but changes shape when pushed and pulled by the air around it. The wind too is never steady. One does not want to stop at understanding how flight would happen in an artificially simplified situation, or build a robot or vehicle that cannot handle a gusty environment.

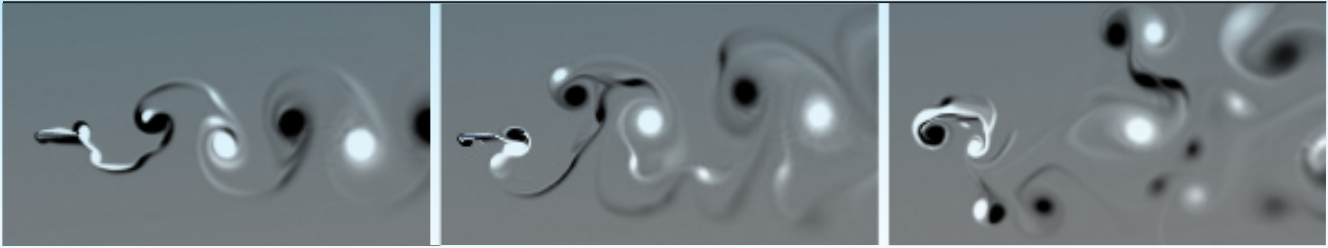
The problem is a daunting one, but as long as it can be broken into stages of increasing complexity, it is a problem that can be attacked. Dr. Sarkar, Chandan and Sandeep Badrinath (then a Dual Degree student) started with a single, repetitive, plunging motion, and found a wealth of interesting results even in this simplified model. First, they assumed that the air would have a constant density throughout the simulation, meaning that their theoretical model would ignore any compression of it. They then observed what happens when flapping becomes more and more rigorous, and tried to understand and explain it.



A low-speed wind facing a small flapping wing would behave the same way as a wind of twice the speed facing a wing either double the size, or one flapping twice as fast. It would be as if the entire system had been scaled up or down (suppose each of us were to shrink to the size of ants, if everything around us shrank by the same scale, no one would ever notice). This is why it is common practice to use the non-dimensional form of the NSE, that is, all lengths are divided by a characteristic length (such as the wing span), all times by a characteristic time (such as the duration of one flap), and so on. This gives us an equation involving numerical parameters which have values but no units. Loosely speaking, these parameters, by occurring in different terms of the NSE, decide which terms dominate and thus how the system behaves. One such parameter is the Strouhal number, important in periodic systems such as these. It is the product of frequency (how often the wing flaps) and amplitude (how much it moves in each flap), divided by the wind speed. So, to study a system with an increased Strouhal number, flapping harder or flapping faster would have the same effect. However, changing the flapping frequency would affect the ability of the numerical solver to find solutions, unless the time step was also altered suitably, so the researchers chose to change the amplitude to see what happened, knowing that all that mattered was the overall change in Strouhal number.

When a wing does not flap, the air flowing past it keeps close to its edges, flowing smoothly along them. Flapping changes this. At first, the wing flaps softly, moving only slightly every time. The air in its wake swirls around, forming what are called vortices. The vortices form just as regularly as the flapping, making the same





*Vorticity contours in the wake of the flapping wing for (left to right) periodic, intermittent, and chaotic cases.*

pattern as each cycle repeats. As the range of motion of the wing grows, however, something interesting begins to happen. The vortices repeat for a while, and move around unpredictably for a while before they begin to repeat again. As the flapping amplitude grows larger and larger, these intervals or “windows” of unpredictable behaviour begin to grow until the entire behaviour becomes unpredictable.

Once this has happened, if one were to take a picture of the flow field at some time, and superpose it on the original flow field, one would get a blurred image, even if the wing was at the same stage in its flapping cycle. This gives researchers in the field a hunch that the system has become chaotic. However, there is a rigorous mathematical definition for chaos. Establishing that this is indeed chaos, deciding how chaotic it is, and being sure that it transitions from well-behaved repetitive behaviour to chaotic behaviour via an intermediate state of “intermittency”, as the growing windows of unpredictability seem to show, is not a trivial task. Since the equations involved are a set of non-linear partial differential equations that are solved by creating a mesh of tens of thousands of cells, the numbers being different at each point in time and space, some of the tools most widely used to establish chaos turn out to be poorly suited to these studies. To identify the behaviour as chaos, Sandeep used a technique based on the idea that when some property of the system is observed at two instants some time apart, the extent of correlation between the two should describe how periodic the system is. A system that is periodic would keep coming back to its initial state, unlike a chaotic one.

To study how the originally periodic system becomes chaotic over time, the researchers used a different tool, called recurrence quantification analysis, which shows, in a single plot, the tendency of a system to repeat its behaviour. This gives a visual intuition, like the pictures of vortices in the wake of the flapping wing, but also allows quantitative measurements. Since recurrence analysis leads to results that can be used to measure periodicity, it is useful for identifying the moment when a system begins to show irregular behaviour.

The brains of flying animals use highly advanced control strategies to deal with all kinds of air flows, but if we were to build a robot to fly like an insect or a bird, and endow it with a small circuit to control its flapping based on how much lift it was receiving from the air, we would very much like to avoid setting up unpredictable flow fields and losing control of the flight.

The next step in Chandan’s work has been to complicate the system even further, to bring it closer to reality. Just as the flapping wing has an effect on the air, the air has an effect on the wing. He started by forcing the wing to move in a way that had already been determined, regardless of the forces from the air. This is called a kinematic model, because it concerns itself with only the motion of the wing; the theoretical wing in the model does not respond to lift, drag and so on. He now moves to a dynamic model, allowing the mass and the stiffness of the wing to affect its behaviour in the flow. Of course, this means he must stop dictating the flapping, and let the forces dictate it instead. He sets off the system with a tap and then watches what happens.

To be able to watch what happens, he needs an enormously complicated piece of code. The physics has now come full circle, from the flapping of the wing determining the flow, to the flow pushing the wing around. To handle these two aspects, he now needs two solvers. At every instant, the wing has a certain configuration. With this





information and the wind speed, a Navier Stokes solver finds the pressures at different locations in the flow. This information is given to a Fluid-Structure Interaction solver, which computes the effect of the pressures in the air on the wing, by creating special kinds of meshes on both the fluid and the structure, and carefully ensuring that their interaction is accurately represented by the equations. This tells the NSE solver the new configuration of the wing, so that the latter is ready to move on to the next time step.

This time, he includes both pitch and plunge, making the wing tilt periodically in addition to moving up and down. To start with, the wing is treated as a combination of a block, representing its mass, and a spring, representing its stiffness. This kind of approximation is called a lumped mass model, and is very useful for modelling physical systems in a basic sense. His intention is to move on to three-dimensional motion and use a finite element model, in which the wing would be treated as a large number of tiny connected elements, bringing the theoretical model closer to a real wing.

It is a never-ending search for the truth, but that is what scientists do. It is also a never-ending effort to be creative with whatever glimpses we have of the truth — that is what engineers do. Scientists cannot give up on the hope of understanding how nature works; engineers cannot allow limited understanding of nature to stop them from making things. These researchers are both, using whatever tools are at their disposal to either break problems open, or peel them apart layer by layer. It would be difficult to decide which would be more exciting: the prospect of seeing tiny flying machines with flapping wings doing reconnaissance work for us, collecting data humans cannot collect, from places where humans cannot go — or the prospect of finally, having watched nature tease us for all this time, truly understanding how birds and insects fly. Whether or not we shall ever be able to beat nature at her own game, every step we take to understand these strange and wonderful systems brings us closer to figuring out the rules.



*Prof. Sunetra Sarkar's team*



***Shivani Guptasarma*** (Author)

Shivani is a fourth-year undergraduate studying biomedical engineering at the Department of Engineering Design, which means that she is engaged in an endless but pleasant effort to master many fields. She is particularly interested in mechanisms and manipulators, imaging and image processing, and medical and assistive product design.



***Dr. Sunetra Sarkar*** is an Associate Professor in the Department of Aerospace Engineering. Her broad areas of interest are aerodynamics of micro-air-vehicles (MAVs), fluid-structure interaction problems, and aero-elastic instabilities.



## *Unraveling Uncertainty*

by *Nikhita Damaraju*

*U*ncertainty is present all around us, from the change in climate around the world to the oscillations of nerves in the nerve-muscle junction. Observing the uncertainties in wing oscillations could help with devising early warning systems to make safer aircrafts.



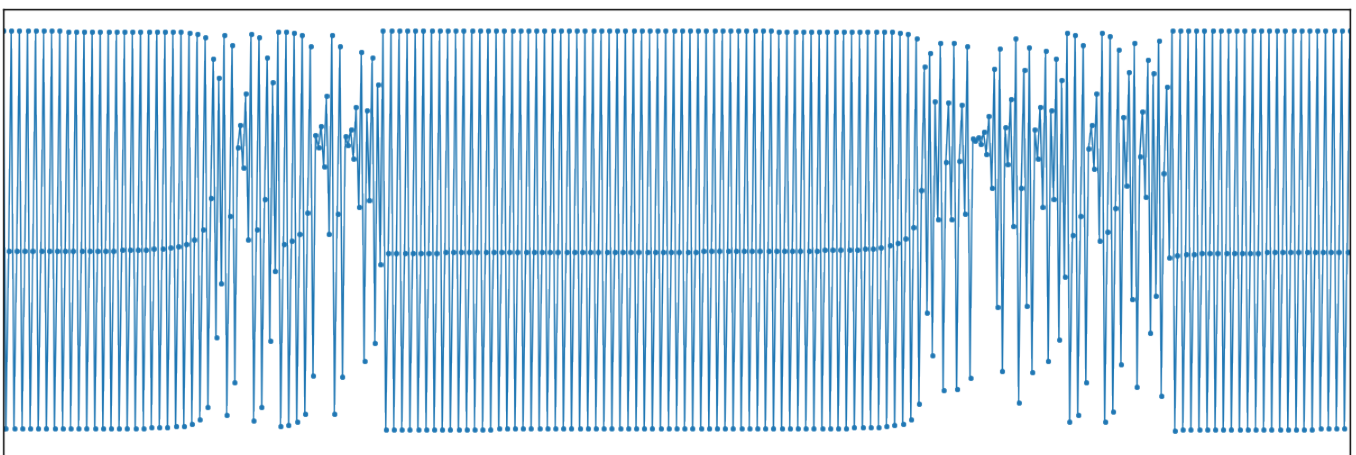


The term uncertainty strikes us as something that is not predictable or definite. When mechanical systems are designed, a lot of idealisations are made - mathematical models used to represent these systems are not exact representatives of their behavior in real life. This is due to the presence of uncertainties or states of randomness. Dr Sayan Gupta's lab - "The Uncertainty Lab", in the Department of Applied Mechanics, is dedicated to exploring uncertainties in modelling various systems inspired from real life. Dr Gupta and his students study the behaviour of systems when under the influence of uncertain forces. He remarks about the name of his lab, saying, "It's not an uncertain lab. It's an uncertainty lab!"

Dr Gupta's work is highly collaborative and interdisciplinary, as he often works alongside Dr Sunetra Sarkar of the Aerospace Department and Dr Shaikh Faruque Ali of the Applied Mechanics Department, among others. Uncertainty arises due to the ignorance of the random or stochastic nature of a system in real life. Dr Gupta points out that "everything is uncertain". During the modelling of a system, idealisations bring in a lot of errors. It is therefore, not clear whether the end result obtained is accurate or not. In order to study such behaviour, there needs to be some kind of mechanism to know how a stochastically or randomly varying parameter affects a system's response.

S Krishna Kumar, one of Dr Gupta's PhD students, studies and models how randomness in wind flow affects the movement of the wings of an airplane, modelled using an airfoil. The kind of study that he does can also be used to understand the complications in modelling other systems, like a bridge or a skyscraper. He explains to us that an aircraft wing system has two states - static and oscillatory. As the name suggests, in the static state, the aircraft's wing is considered to be at rest, and in the oscillatory state the wing is observed to move vigorously. When the aircraft speed or its angle of inclination are relatively low, the state of the wing is found to be static. As the speed of the aircraft or the incline angle increases beyond a threshold, the "static state" of the wing transitions into the "oscillatory state".

In a realistic model, the static state of the wing is not truly still or stationary. It is modelled as having random fluctuations - this is where uncertainty is an input into the model. To consider the static state as one with fluctuations is, in fact, a very realistic assumption. So, the static state is considered to have irregular behaviour, on account of random fluctuations, whereas the oscillatory state can be modelled as having a definite frequency and amplitude. A transition from the static to a completely oscillatory state is considered to be a transition from irregular to regular behavior. This transition is observed to happen via a series of intermediate states known as intermittencies.



*A time series illustrating intermittency: Coexistence of periodic behaviour and random behaviour*

An intermittent state is a mix of seemingly random and seemingly oscillatory states, as illustrated in the figure above. Intermittency has usually been reported as curious discoveries, and in-depth studies of this phenomena has been ignored for a long time.



In the system of interest for the present study, the vigorous oscillations observed in the airfoil are called “flutter”. Aircraft wings are thin, slender, and light structures, and thus cannot withstand these vigorous oscillations, which can cause them to break away from the fuselage of the aircraft.

One method to handle this problem is to use controllers to minimize the flutter once it occurs. Controlling the flutter involves applying mechanical techniques to reduce the oscillations once they begin to occur. Krishna Kumar tells us that controllers are present in most present day aircrafts.



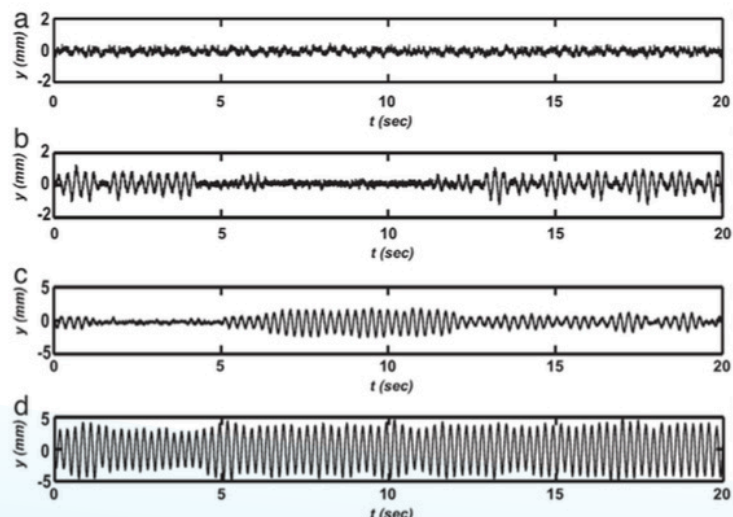
The alternative, which is what Dr Gupta has worked on, is to predict the onset of flutter in order to remain in a safe flying regime. Krishna Kumar tells us that they want to identify precursors before the onset of flutter. At low speed of the aircraft, the wing is almost static, or has small or weak oscillations that eventually decay. Once the flow speed past the wing increases past a critical value, the airfoil oscillations cross a threshold, and cannot be ignore. With a further increase in these oscillations due to high speed of the aircraft, these oscillations become more dominant and vigorous. The natural question to ask is - at what speed should one fly an aircraft so that flutter does not occur?

“Theoretically, this sounds very simple”, Krishna Kumar says. He explains that an aircraft model can be tested to find the critical value of this transition, and extrapolating to real life situations, speeds past this critical value can be avoided. However, the simulations of wind flow and aircraft speed in a controlled laboratory setting are very idealistic. In reality, these factors continuously fluctuate. For example, the speed of an aircraft varies based on external environmental conditions like wind speed and extent of cloud cover.

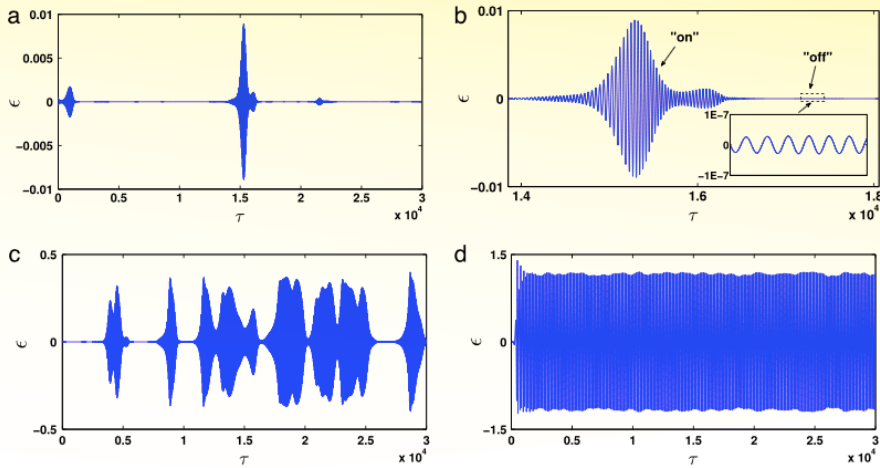
So, as part of their work, Dr Gupta and his students find precursors before the wing begins to flutter. These precursors are the intermittent states that occur during the transition from the randomly fluctuating and the oscillatory state. The idea is that if one can measure the presence of intermittency (which occurs well before flutter), it can serve as an early warning signal.

Dr Sayan and his students have carried out wind tunnel experiments, as well as numerical studies, to study how an airfoil behaves in different wind flow regimes. They observed that as the flow speed past the airfoil is increased, there were intermittent bursts of periodic oscillations amid the background of random fluctuations. As the flow speed in increased further, the intermittent bursts of oscillations last longer, and soon the behaviour of the airfoil transitions to fully developed periodic oscillations (or flutter).

*Airfoil plunge response from experiments done by Dr Gupta's group, with increasing flow speeds from (a) to (d), showing a transition from random fluctuations to fully developed periodic oscillations, via intermittent stages.*

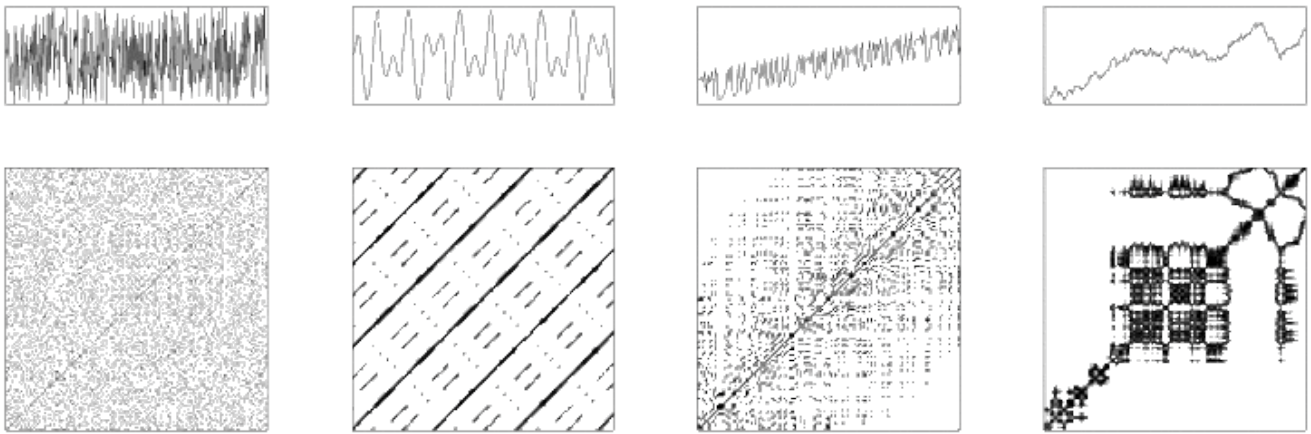






Plunge response of airfoil in the presence of fluctuations, from numerical calculations carried out by Dr Gupta's group. Flow speeds increase in the order of (a), (c), and (d), showing corresponding increase in frequency of periodic oscillations, until fully developed oscillations are observed. (b) is a Zoomed-in view of (a), highlighting the on-off intermittency.

In order to study the intermittent states, a mathematical tool called the recurrence plot is used. This tool picks up whether a system exhibits regular, irregular, or intermittent behavior. As the name suggests, this tool looks for recurrences, or repetitions, in the system's dynamics.



Different time series with corresponding recurrence plots.

A recurrence plot of a given time series of length  $N$  is a matrix of dimension  $N \times N$  (see image above). The  $ij$ th element in this recurrence matrix indicates whether the state of the system at time  $i$  was similar to the state of the system at time  $j$  - if it was, then the corresponding element is shown with a black dot in the plot.

An irregular system appears grainy in the recurrence plot - without any clear pattern or message about the original data used to draw the plot. Whereas, for a regular system, its recurrence plot shows repeated structure. For an intermittent system, the recurrence plot has a mix of both repeated structure and grainy structure. This structure, or lack thereof, can be captured using some mathematical measure calculated on the recurrence matrix, and the irregularities or regularities can be captured and quantified. The changing values of irregularities to regularities can thus be used as a precursor to flutter in the aircraft wing.

Dr Gupta and his students want to go beyond devising effective warning methods using intermittency. They also want to understand why the phenomenon of intermittency occurs. Dr Gupta tells us that it is interesting to note that intermittencies are also seen in other physical systems - like sunspot data in solar flares giving information as to when sunspots occur, nerve oscillations in muscles, and many more.

Krishna Kumar adds that once they understood that the randomness, or uncertainty, was what drives intermittency in many systems, they started exploring the possible mechanisms involved. Among many things, they found that the nature of the intermittency depends on the time scales governing the input. In other words, for their airfoil system, the type or pattern of intermittency depends on the nature of the flow velocity. If the flow

velocity varies rapidly, it causes 'burst type intermittency'. However, when it is slowly varying, it causes 'on-off intermittency'. Both these types of intermittencies have same origin, but they show up differently in the output behaviour. This kind of understanding of intermittency can help prepare more robust and practically useful precursors, among other applications.

To conclude this journey into understanding the world of uncertainties, we are certain of a few things. One route to chaos is through states of intermittency, and understanding this uncharted region helps us pick precursors in order to devise early warning systems.



***Nikhita Damaraju*** (Author)

Nikhita is an third year undergrad from Biological Sciences. She aims to probe answers to questions in the field of Cancer Biology using Data Sciences. Aside from this, she loves playing the violin, running and listening to Carnatic Music.



***Dr. Sayan Gupta*** is an Associate Professor in the Department of Applied Mechanics. His research interests lie in the field of stochastic dynamics and structural risk assessment.

He broadly focuses on nonlinear dynamics, probabilistic mechanics, stochastic load modeling, structural reliability and life prediction, structural system identification and health monitoring from vibration measurements, and energy harvesting from wind.



## *The Real Master of the Brain : **Glia** ?*

*by Sherlyn Jemimah*

*F*or decades, researchers working on neurodegenerative disorders (like Parkinson's and Alzheimer's) focused on figuring out what happens in the neurons (brain cells). Brain research is replete with molecular and system-based studies, with neurons as the centerpiece. Now, data from next-generation sequencing technology has shed light on a group of cells, often overlooked in research, which may hold the key to fighting neurodegenerative disorders.



Neurons are specialized cells in the nervous system, tasked with transmitting information to neighboring neurons, muscle or gland cells. They consist of a cell body, an axon and dendrites, the ends of which contain synapses (connections to other cells). Neurons are essential for our brain's functioning: for instance, as you read this article, your neurons transmit electrical impulses, or "fire" in different regions of your brain, allowing you to recognize words and process information. Virtually all our activities, be it walking, talking or thinking, is enabled by neurons.

### **Neurodegenerative Disorders**

Due to their importance, the loss of neurons through cell death or damage manifests as problems in mental functioning: a loss of memory, motor skills and/or cognitive skills. These problems are grouped under the term neurodegenerative disorders. The type of disorder depends on the type of neurons affected. For example, in Parkinson's disease (PD), the SNc (substantia nigra pars compacta) neurons in the basal ganglia region (which controls bodily movement) of the brain are affected first, followed by other neurons in higher cortical regions. This is correlated with symptoms which include unwanted limb movements, and in later stages, memory problems. In Alzheimer's (AD), the hippocampal neurons in the temporal lobe of the brain are affected first, followed by other regions of the brain. This is seen in the initial stage as problems with short-term memory, followed by a loss of motor control. Doctors note that the first symptoms of PD and AD manifest at approximately 60 - 65 years of age, when around 50 - 60% of the neurons have died. However, the warning signs of sleeping problems, constipation problems, low libido and/or a diminished sense of smell are often seen at 35 to 40 years, when the neurons presumably start to die. Treatment options are limited and focus on relieving the symptoms of the disease. Neurotransmitters (like acetylcholine for AD and dopamine for PD) are found to be at low levels and are therefore supplemented through medication: levodopa or acetylcholine. Patients often overdose on the medication to feel 'better' for longer, and do not take it regularly as prescribed by their doctor. In the long term, this causes the aggravation of dyskinesia (uncontrollable limb movements), the very symptom it was intended to prevent. At this point, patients need expensive deep brain stimulation to alleviate their worsening condition.

Neurodegenerative disorders affect approximately 45-50 million people worldwide. PD affects around 1% of the global over-60 population. In India alone, it is estimated that over 7 million patients suffer with PD. The age-specific prevalence of PD is estimated to be 76 to 148 per 100,000 in India. Certain ethnic groups seem to be affected disproportionately, pointing to a strong genetic component in the illness. A study on the Parsi community in Mumbai showed a prevalence of 328 per 100,000. In the case of Alzheimer's, there are an estimated 4 million patients in India, with the number of cases expected to double by 2030. Neurodegenerative diseases not only affect the patients, but also their families, who face added stress and anxiety due to behavioral changes exhibited by the patients, resulting in emotional and social costs, apart from the financial cost of treatment. On a positive note, the prevalence of neurodegenerative disorders is much lower in India compared to global statistics. However, due to the large, rapidly ageing population, the disease burden in India is high.

### **NGS Data Analysis**

Certain types of neurons are more vulnerable in neurodegenerative diseases. For instance, consider SNc neurons in PD. These neurons are dopaminergic, which means that they are the source of dopamine, an important neurotransmitter associated with movement, memory and reward-based behavior. Although the brain harbors other types of dopaminergic neurons (such as ventral tegmental area neurons), only SNc neurons are affected in the initial stages of Parkinson's disease. A similar phenomenon is observed in AD as well, with hippocampal neurons affected first.

*What makes this neuronal subpopulation vulnerable?*





To find a concrete answer to this question, Dr. M. Michael Gromiha and Akila Parvathy Dharshini S, a Ph.D. scholar at the Protein Bioinformatics Lab, decided to work with next-generation sequencing (NGS) transcriptome data, in collaboration with Prof. Y-h. Taguchi of Chuo University, Japan. Akila also had a number of discussions with Prof. Srinivasa Chakravarthy, head of the Computational Neuroscience Lab.

NGS data analysis was chosen for its potential applications in personalized medicine. NGS refers to the highly efficient, revolutionary technique of sequencing the genome (i.e. the entire DNA sequence of any organism). In this technique, the DNA of the organism is split into millions of fragments, which are then multiplied millions of times using a chain reaction. Each fragment is therefore read millions of times, eliminating any reading errors. The individual fragments are then pieced together using advanced software. It is considerably quicker, cheaper, highly reliable and more accurate than other sequencing techniques. NGS data is available in public repositories, including NCBI's SRA (Sequence Read Archive from the National Center for Biotechnology Information).

What is the transcriptome, and why do we use it? A transcriptome represents the sum of gene transcripts in a given cell/tissue sample. Genes are made up of DNA sequences, a biomolecule made up of 4 nucleotide bases represented by the letters A (adenine), G (guanine), C (cytosine) and T (thymine). So, DNA (and therefore, the gene) consists of a long sequence of A, G, C and T. In all cells, genes have to be transcribed into another biomolecule called RNA before they can be used to make proteins. RNA (ribonucleic acid), like DNA, is a sequence of A (adenine), G (guanine), C (cytosine) and U (uracil instead of thymine, T). So, gene transcripts are essentially the RNA version of the genes. Why are gene transcripts important? In every cell, only certain genes may be transcribed, and some genes may be transcribed more often than others. This is why, a neuron is very different from skin cells, both in terms of appearance and its internal working. While a neuron and a skin cell from an individual will have the same DNA, their transcriptomes will be vastly different. Transcriptomes are more useful when comparing patients with healthy individuals, as they can be used to identify differences which would otherwise be missed if we just compared their DNA.

Akila worked with transcriptome data taken from the temporal lobes and frontal lobes of patients in the advanced stages of Alzheimer's disease as well as healthy subjects. Three types of analyses were carried out on the data: SNP (single nucleotide polymorphism) analysis, differential gene expression analysis and network analysis. SNP analysis finds single-letter differences between the patients and healthy individuals. In differential gene expression analysis, differences in gene transcription are studied. The differences were then mapped to the products of the genes, i.e. proteins. From these proteins, the affected pathways (which can be understood as a set of proteins performing a related function in the cell) are identified. Thus, an accurate snapshot of the affected cells could be constructed from the variations present in the transcriptome data.

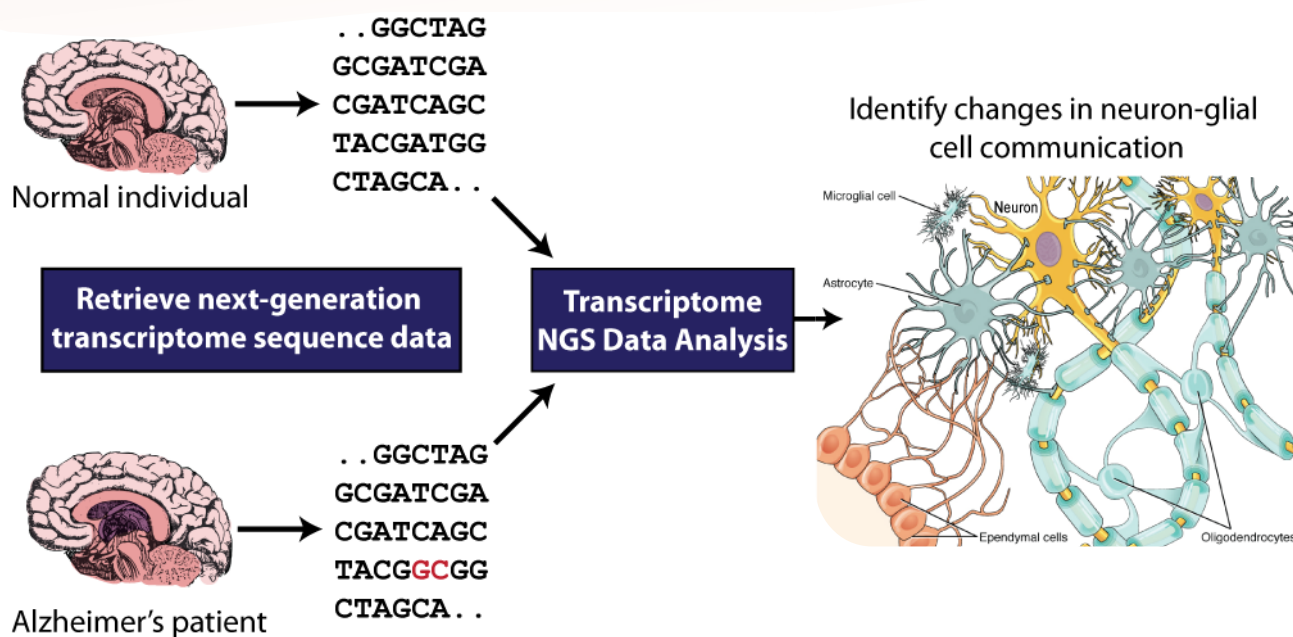
### **Major Findings**

Decades of research have uncovered many possible contributing factors in neurodegenerative disorders, including energy imbalance, calcium load and protein aggregation. These studies focus on the neurons, and this is understandable for two reasons: scientists presumed that the problem was in the neurons, and neurons are easy to study because their electrical activity could be measured easily. However, the transcriptome data analysis suggests that glial cells, not just neurons, may be vulnerable in neurodegenerative disorders.

Glial cells (also referred to as glia or neuroglial cells) constitute a significant percentage (60 - 80%) of the brain and spinal cord. The word "glia" comes from the Greek word for "glue", from the belief that these cells hold the brain together in some way. They come in four distinct types: astrocytes (star-shaped, hence the name), which maintain the chemical environment of the neurons; oligodendrocytes, which wrap the neurons in a myelin sheath; microglia, which remove cell debris, much like a macrophage engulfing a pathogen; and NG-2 glia, which generate new oligodendrocytes and regulate the synapses between neurons. Additionally, glial cells supply energy to the neurons by acting as a go-between for the neurons and the blood vessels. Neurons "tell" the glial cell how much

energy they need, and the glial cells obtain this energy from the bloodstream, convert it into lactate, and transport it to the neurons. In fact, 60-70% of the energy needed by neurons comes from glial cells. The importance of glial cells - the *other brain*\* - has only been realized in the past 3-4 years.

Energy imbalance has been cited as a cause for neuron cell damage and/or death in PD. Insufficient energy supply may result in cell damage and death. NGS data analysis shows that glial cells associated with vulnerable neurons seem to lose their structural integrity, and consequently could not keep up with the energy demands of the neurons. It also identified a communication gap between the neurons and the glial cells; the neurons were no longer able to tell the glial cell how much energy was needed.



*NGS transcriptome data analysis at a glance: Finding out the real cause of neurodegenerative disorders.*

### The Road Ahead

The NGS data analysis hints at the role of glial cells in neurodegenerative disorders and may provide clues to answer questions on the selective vulnerability of the neurons. The research work is due to be published soon. As with most diseases, emerging evidence suggests that our lifestyle choices (in terms of diet, exercise and mental stimulation) play a prominent role in lowering the risk and delaying the onset and progression of neurodegenerative diseases. Various studies correlate regular physical activity with improved neuron health. Learning multiple languages may also help delay the onset of the disease. For patients and their families, good coping strategies include learning about the disease, physical therapy and involvement with support groups. A healthy lifestyle is key to overcoming neurodegenerative disorders.

\**The Other Brain: The Scientific and Medical Breakthroughs That Will Heal Our Brains and Revolutionize Our Health* is a highly acclaimed scientific work by **Dr. R. Douglas Fields**, detailing the role of glial cells in neurodegenerative disorders and everyday neuron activities. It is published by Simon and Schuster.



**Sherlyn Jemimah** (*Author*)

Sherlyn Jemimah is a research scholar at the Department of Biotechnology, IIT Madras, and works on the computational analysis of mutant protein-protein interactions. When she is not doing research, she devours popular science articles and enjoys playing music.



**Dr. M. Michael Gromiha** is an Associate Professor at the Department of Biotechnology, IIT Madras and heads the Protein Bioinformatics lab. His research interests include protein stability and folding, protein interactions, protein aggregation, mutation studies, structure-based drug design, deep learning and NGS data analysis. He obtained his Ph.D. in Computational Molecular Biophysics from Bharathidasan University, India in 1989. His post-doctoral experience includes the International Center for Genetic Engineering and Biotechnology (ICGEB), Italy and the Institute of Physical and Chemical Research (RIKEN), Japan. He has also served as a Senior Research Scientist at the National Institute of Advanced Industrial Science and Technology (AIST), Japan. You can learn more at <https://www.iitm.ac.in/bioinfo/Gromiha/index.html>.



*Prof. Gromiha's team*





# COMBATING WATER CRISIS

## *A Versatile Approach to Sustainability*

by Kanka Ghosh & Priya Khola

*The challenge of having to work with limited resources has been the driving force behind several technological innovations in the past. Today, the need of the hour to develop sustainable solutions for the present and future generations is even higher as the pressure on water resources increases rapidly by the hour.*

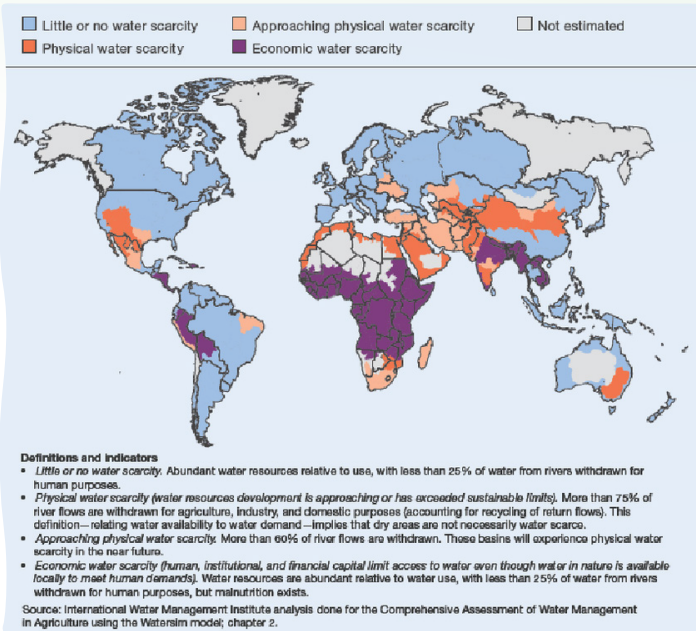
*Prof. Ligy Philip and her enthusiastic group of research scholars in IIT Madras are fighting tooth and nail to resolve some unavoidable facets of water-management which has a direct bearing on the wise utilization of water resources at hand today.*





### Why bother with waste water?

United Nation reports estimate that globally, around 783 million people<sup>[1]</sup> do not have access to clean water. In 2010, the United Nations General Assembly recognized access to water and sanitation as a human right and yet we find ourselves continually haunted by physical and economical<sup>[2]</sup> water crisis with an ever-increasing sense of insecurity. A more recent, WHO- UNICEF report (2014) emphasized that 946 million people globally, still practice open defecation which in turn gives rise to several waterborne and vector-borne diseases such as cholera, diarrhea, jaundice etc.



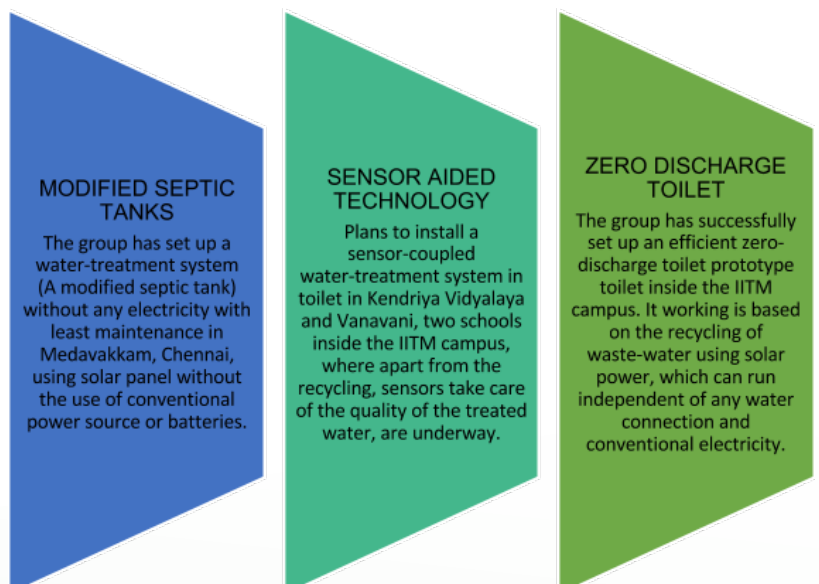
*Physical and Economic water scarcity data from International Water Management Institute analysis*

In India, too the situation is quite miserable. It has been reported that 626 million people in India don't have proper toilet facilities in households. Another report, based on data from the Ministry of Urban Development (2013) and Central Pollution Control Board, estimates that 75-80 % of water pollution results from domestic sewage and that untreated sewage flowing into water bodies such as rivers has almost doubled in recent years. More alarmingly, in a recent study, WHO/UNICEF Joint Monitoring Program (JMP) for Water Supply and Sanitation has released a ranking of the countries based on an estimate of improvement of sanitation facilities in a time duration between 2000-2015 where India ranks 154 out of 188 countries<sup>[3]</sup>. In these circumstances, waste-water management is crucial towards providing a sustainable solution.

### A Decentralized Route for Sustainability

In ensuring the safe & smooth distribution of resources in a community, wastewater management has always been a challenging undertaking. This is because the outcomes of doing so not only affects the health of the community, but also determines the efficiency of the utilization of water as a scarce resource. Therefore, there is a need for responsible management of waste-water. One of the prominent problems regarding the wastewater management is the modus operandi of the traditionally installed centralized sewage systems. The problems associated with it are manifold in nature. In a centralized sewage treatment system, wastes are collected through the pipeline which connects the centralized treatment plant to the sewer system. In Chennai, there are 6 centralized plants, which collect wastes throughout the city. Transport operations incur high costs and difficulties arise since wastewater is recycled far from where it was collected.

Dr. Phillip along with her scholars from EWRE (Environmental and Water Resources Engineering) division of Civil engineering department have undertaken an alternate decentralized route to resolve these issues. The concept of decentralized sewage-treatment is slowly coming to the front for the need of recycling of water. Prof. Ligy's group involved in developing different techniques for decentralized systems.



Prof. Ligy provided rough estimates on the amount of water they are recycling at the IITM wastewater plant, located near the IIT Madras Research Park. "Daily, we save 8-10 lakh litres of water inside our campus!", she smiled confidently. Her estimates gave us a glimpse of the magnitude of the problem they are trying to solve. We discuss some of the notable activities of Prof. Ligy's group in detail in the next section.

### **Bacteria & Bio-digesters**

Started in September 2015 and funded by the Bill and Melinda Gates Foundation is a project titled 'Monitoring and Evaluating the Onsite Waste-Water Treatment System Comprising of DRDO Based Anaerobic Digestion Units for Toilets in South India.' It is one of the many projects Prof. Ligy Phillip and her research scholars have been working on. Anaerobic digestion is a series of biological processes in which microorganisms (mostly bacteria) break down biodegradable material in the absence of oxygen. These anaerobic digesters are employed in waste-water treatment plants



*Inoculum bacteria*

to break down sewage residues and eliminate pathogens in waste-water. Likewise, the digester units deployed in this project are essentially modified septic tanks. A biodigester is like a mechanical stomach. It is fed with organic material, which is broken down (decomposed) by microorganisms (bacteria) in an oxygen-free (anaerobic) environment to produce a renewable energy called bio-gas (methane and carbon dioxide) and other material that is mainly used as fertilizer. Since all the starting material used are organic, break down of these organic moieties results in simpler organic molecules.

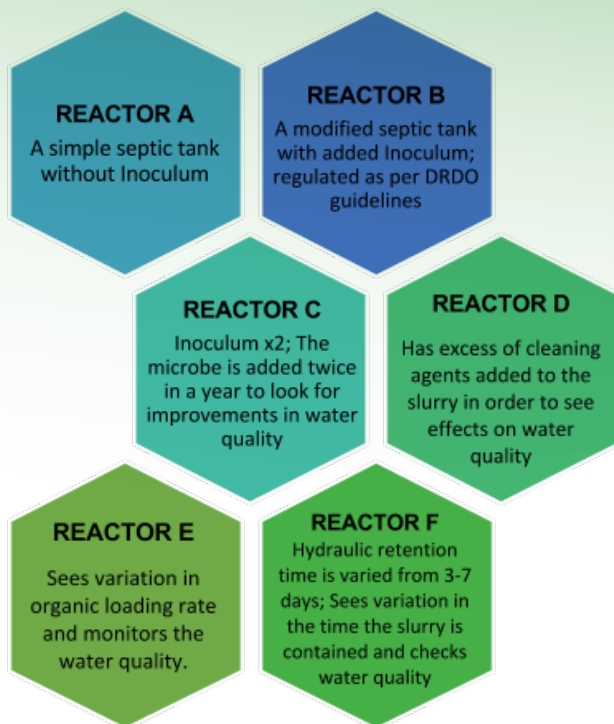
Septic tank systems are a type of onsite sewage facility (OSSF). They are watertight chambers made of concrete, fibreglass, PVC or plastic, through which sewage flows for primary treatment. Water is allowed to stand for a given settling time and later anaerobic processes reduce solids and organics. But the treatment is only moderate and they are used in areas that are not connected to a sewerage system, such as rural locations.

The modified septic tank comes with three compartments with a scrub resembling material forming the base of the tank which increases the activity. It is a microbial consortium a mixture of different bacteria in a fixed composition called Inoculum. The microbes feed on the fecal matter and hence reduce the carbon and nitrogen components into simpler molecules. This technology has been patented by DRDO and as per their claims, Inoculum once added to the biodigester, is enough for a lifetime. As Dr. Kalai Vani, a research scholar at Prof. Ligy's lab explains, DRDO makes these anaerobic bio digesters for the treatment of black water i.e. the water which comes out of the toilets and has been able to achieve up to 60-65% treatment efficiency with respect to organic matter removal. This performance is comparable with a septic tank without any inoculum addition. Presently, biodigesters placed in 13 sites across South India are under evaluation with one of the sites being here, at IIT Madras. In order to unearth the science surrounding this innovation, we ventured forth to ask the procedure for evaluation of the biodigester, to which Dr. Kala Vani very patiently explained that they had installed six reactors namely *A*, *B*, *C*, *D*, *E* and *F* at different locations in the lush green IIT campus with each one being operated under different conditions:



*A typical real-time bio-digester*





### ***Running a Decentralized Sanitation System***

Next, we had the opportunity of speaking with Mr. Ram Prasad, one of the research scholars in the team who spoke to us about his project

- a community-based waste-water management system being carried out in Medavakkam. Obtaining the project requirements begin with the collection of black and yellow water from 264 households followed by their treatment. The waste-water is treated using the modified septic tank which has a baffled reactor installed in it. This septic tank is in anaerobic condition initially and so the dissolved oxygen (DO) level is very low.

In anaerobic tanks, most of the solid is retained and then further degraded by microbes. Oxygen is then provided to the system by means of diffused aeration. Following aeration, air is blown from bottom so that the system is enriched in oxygen. Until this stage, it is expected that most of the solid must have been degraded by the microbes in the baffled reactor. After the anaerobic unit, an aerobic unit is provided to further clean the water. A pressure pump is utilized in the next step in which sand acts as a filter so that the leftover solid particles will be filtered through sand. It starts working automatically once contents in the tank reach a certain volume. This pump will backwash the sand as well. This whole process from baffled reactor to the filtering of water is automated. Finally, the water is sent in for chlorination.

This simple septic tank is capable of recycling 2600 litres of water everyday. Recovery percentage lies between 80-90% and the whole setup costs less than 5 lakhs! Owing to the hours need to become environment friendly, the system is designed to run entirely on solar power.

On the whole, this anaerobic bio-digester is energy efficient as well as cost efficient. Residents of Medavakkam responded with positive reviews saying they were quite happy with the quality of water and were pleased to recycle and reuse the water, thus displaying their faith in this new technology. Back in campus, a modified septic tank with sensor, is in process of being installed in KV school. The sensors, one at the inlet and the other at the outlet will check the quality of water by measuring values for turbidity and dissolved oxygen (DO) levels. If the quality of water isn't found to be up to the mark, it will be drained out to the soak pit for further treatment.

In order to routinely monitor the working of the biodigester, the team collects samples from each reactor and tests them in the lab by different techniques. These techniques measure the pH-levels, temperature, dissolved oxygen, ammoniacal nitrogen, fecal coliform and many more constituents by different laboratory techniques. Ground level monitoring results show a removal efficiency of 60-65% against the values of 80-90%, claimed by the vendors.



*FRP bio-digester used by DRDO license.*

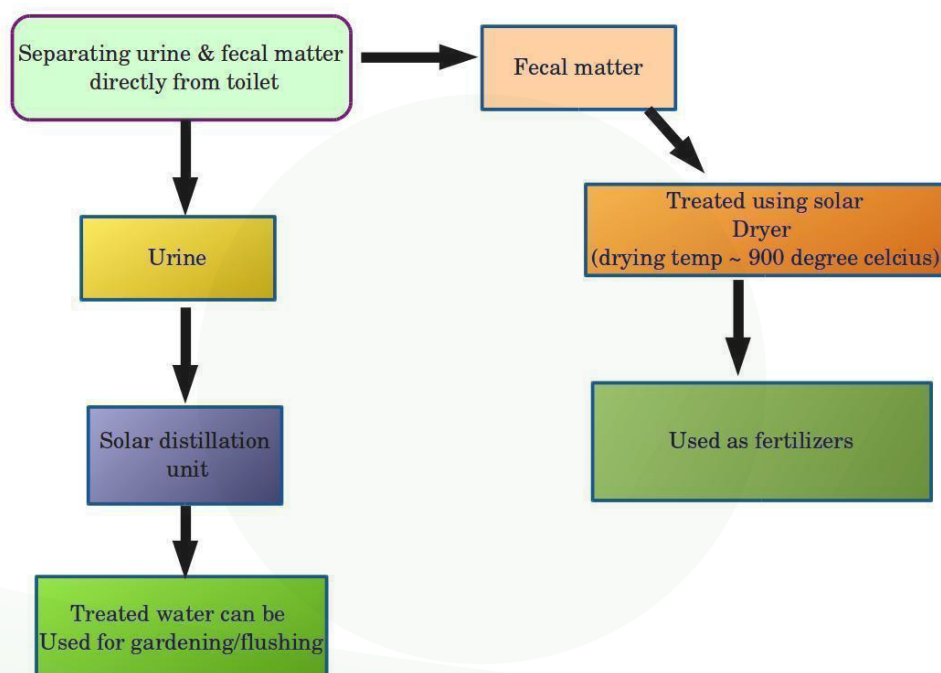


*Photographical view of on-site waste-water treatment.*

### **The Zero- Discharge Toilet**

In association with Prof. K.Srinivas Reddy from the Mechanical Engineering Department, the idea of zero-discharge toilet emerged from Dr. Phillip's group. Research scholar Krithika, an active member in this project, tells us about the usefulness and functionality of these kinds of sustainable development technologies in our society. Amidst the erratic power supply, lack of funds and skilled personnel, it is a challenge to look upon wastes from wastewater treatment plants as a resource even after putting it through rigorous treatment.

Composition-wise, black water (waste-water containing feces, urine) is very different from grey water (waste-water generated from shower, baths, washing). Krithika adds, We can't combine black water with grey water as black water has more pathogens and it is also rich in nutrients. Zero-Discharge toilet is a manifestation of sustainable treatment of black-water using renewable energy sources. The crucial challenge before the team was to find out means to use black water as fertilizers by extracting its nutritional value. The working principle of zero-discharge toilet consists of several steps showing below:



*Working mechanism of zero-discharge toilet: separating solid and liquid part of the black-waste-water.*



There are plenty of advantages in installing a zero-discharge toilet. First, it is very cost-efficient as there is no external electricity supply to it. Second, since it solely depends on the solar power for distillation, it can easily overcome the problem of inconsistent power supply. Third, the automated system eliminates the need for a centralized wastewater treatment plant and related transportation and maintenance costs.

The project kicked off with studying a lab-scale setup to properly understand and monitor the effectiveness of the methods devised to run the system. The pilot scale system comprised of:

1. **Data Logger** – For online monitoring of ambient and instrument temperature.
2. **Pyranometer** – For the measurement of Intensity of Solar radiation.
3. **Separator With Conveyor System** – For separation of solid and liquid wastes.
4. **Inclined Photo Reactor** – For converting untreated urine into condensate.
5. **Solar Photodryer** – For converting solids fecal matter into soil conditioner.

Synthetic urine and fecal matter had been used as samples for treatment. After separating the solid and the liquid from the waste, the liquid goes to the pump and then passes through the inclined solar photo-reactor unit. The inclined solar reactor gets more sunlight and the excess heat evaporates the water content in the urine and helps the untreated urine to condensate. Then, the treated fresh water is collected. The other part of the waste, namely the solid wastes (fecal matter) are slowly transported to the dryer using a screw conveyor. An inclined stepped photo-thermal dryer is used afterwards. After drying, synthetic bacteria is added to the dried fecal matter which can then be used as a potential fertilizer. The distillation unit was able to achieve almost 90% recovery of water from the liquid waste (urine).

On obtaining encouraging results from the pilot plant, the team finally decided to set-up the real-time zero-discharge toilet. The team has designed and built their very own zero-discharge toilet and it has been installed. The designed system is flexible, compact, stand alone with zero discharge. Moreover, it utilizes solar radiation as the energy source. near the Brahmaputra hostel in IIT Madras.

The field-scale system consists of similar parts used in pilot lab scale setup. The main components that have been used are shown below:



*Real time pilot scale zero discharge toilet at IIT Madras*

The sustainability and the efficiency of the project has been highly applauded and for which the team was felicitated with the prestigious J.C.BOSE-Patent Award.



### The Future of Wastewater Management

“If we don’t plan for long-time solutions we’ll be having plenty of problems.” warns Prof. Ligy Phillip, at the end of our meeting. Though a lot of effort is involved, the awareness on water scarcity and recycling has not penetrated to the ground levels of human society. While the decentralized sanitation system had been embraced long back in the first world countries due to their geographical and demographic characteristics, in India we are far away from applying the concept of decentralization to our sanitation system and realizing its benefits. Prof. Phillip suggests that the regulation surrounding waste and sewage treatment should be more stringent in order to see a positive change come through. This means accounting for every drop of water that forms septage, washing machines, bathrooms and looking for ways to recycle them and ensuring utilization to the fullest.

All things said, technology alone can’t combat water scarcity and sanitation problems. Rather, proper policy and most importantly our awareness regarding these issues should increase to counter the problems. It’s high time to address these issues and set up proper goals for future to eradicate these problems

<sup>[1]</sup> Link : <http://www.un.org/en/sections/issuesdepth/water/>

<sup>[2]</sup> *Physical water scarcity region* : More than 75% of river flows are withdrawn for agriculture, industry, and domestic purposes;  
*Economic water scarcity region* : Water resources are abundant relative to water use, with less than 25% of water from rivers withdrawn for human purposes, but malnutrition exists.

<sup>[3]</sup> Link : <http://www.wssinfo.org/>



#### Priya Khola (Author)

Priya is a second year MSc in Chemistry Department. When not in her lab she can be found watching Rick and Morty and F.R.I.E.N.D.S. An avid reader with interest in Supramolecular Chemistry wants to further do PhD.



#### Kanka (Author)

Kanka is a research scholar working on the molecular structure and dynamics of fluids under confinement in the Dept. of Physics at IITM. Apart from being an avid reader of non-fictions, a crazy movie-buff, an occasional guitarist and a passionate photographer, he often finds solace in travelling with a “Marquez” or a “Jibonanando” or a “Marx” in hand.



**Dr. Ligy Philip** is a Professor in the Environmental and Water Resources Engineering Division of the Civil Engineering Department at IIT Madras. She obtained her B.Tech Degree in Civil Engineering from Mar Athanasius College of Engineering, Kothamangalam (Mahatma Gandhi University, Kottayam). She then pursued Masters and Ph.D in Environmental Engineering from Indian Institute of Technology, Kanpur. Her research interests include Domestic & Industrial Wastewater Treatment, Air Pollution Monitoring, Modeling & Control, Rural Water Supply and Bioremediation of Contaminated Soils, Air & Water.



Prof. Ligy Philip's team



## **SELF DRIVING CARS** *Darkest Secrets Revealed* by Praneeth Srivanth

*Have you ever wished your car to operate on its own after a tiring drive on a highway? Can you imagine a scenario where traffic jams are virtually non-existent? Would it be truly possible to avoid the endless queue outside a parking lot?*

*Here's a sneak peek into the amazing amount of work done in the field of semi-autonomous vehicles by the trio - Dr. Nirav Bhatt, Dr. Ramkrishna Pasumarthy and Mr. Subhadeep Kumar at IIT Madras.*



Advancements in the domain of intelligent vehicles and semi-autonomous cars might soon put an end to the frustrations faced by drivers in conventional vehicles. Let's start with looking at how a person driving a vehicle goes about the whole process in a system without automation. The driver observes cars whizzing past, monitors them through a rear view mirror to get a picture of the traffic condition behind, uses external inputs to apply the brakes at the most appropriate time and accelerates the vehicle if the coast is clear. The primary objective of the whole process is to skillfully navigate the vehicle through the traffic. We might imagine this to be a rather complex task if we were to account for these details and model them. This is at the very core of the challenge that the trio aims to tackle.

As the brains behind such vehicles were designed only by human brains, it comes as no surprise that the semi-autonomous vehicles pretty much mimic what the human driver does. The motion sensors, GPS, LIDAR (Light Detection and Ranging) are the eyes of semi-autonomous vehicles. The control system, image processing algorithms, automatic detection of ambient vehicles constitute the brain of the semi-autonomous vehicles which enable the decision making process in order to charter out proper action plans.

One can see that the coordinated effort that is required in operating a vehicle is as demanding as is required in a multi-instrumental orchestra. The engine has to run properly, the correct amount of brake force has to be applied, the brake force has to propagate and reduce the speed of the vehicle and the wheels have to turn accordingly. In essence there should be no internal discord. If the functioning of all the individual components is accurate, but the system as a whole has a lacuna, then it is akin to the clichéd statement "Operation Successful but Patient Died". Ultimately, just like how a butterfly with thousand eyes would just collapse if its nervous system did not direct it to move in the right direction, the control system has to take up all the responsibility in guiding the vehicle based on the gamut of sensors that populate the vehicle.

### **Self Driving Vehicles – Levels of Autonomy**

<b>Level Zero:</b> No automation	<i>You drive it</i> – acceleration, braking and steering are all controlled by a human driver
<b>Level One:</b> Driver assistance	<i>Hands on the wheel</i> – in certain cases, the car can either take control of the steering wheel or the pedals
<b>Level Two:</b> Partial automation	<i>Hands off the wheel, eyes on the road</i> – In certain modes the car can take over both the pedals and the wheel, but the driver must maintain ultimate control over the vehicle
<b>Level Three:</b> Conditional Automation	<i>Hands off the wheel, eyes off the road (sometimes)</i> – In certain modes, the car can take over the driving responsibilities completely

### **Designing the Control System**

There are two approaches that are commonly used by automobile companies in order to design the control system. One approach proceeds as follows:

1. Several trials are performed in the vehicle training phase wherein vehicles are exposed to a wide range of test scenarios such as traffic patterns, congestion levels, road conditions, etc. Various traffic scenarios, vehicular congestion, traffic signals, wet roads, road blocks, etc. are simulated and the vehicle is trained to perform a certain course of action.
2. After feeding in this data, the vehicle is expected to be 'intelligent' enough to take its own decision in a real-world scenario.

The other end of the spectrum in design is to mathematically model all the possible subsystems of the automobile and then decide on a course of action which would take into account the precise details of the braking, steering and acceleration from a mechanistic point of view.





Both approaches pose various challenges that create complexities during analysis. Industrially, a blend of the two approaches is used with a dominant chunk of the design being based on the data-driven approach. While that might be sufficient from an operational point of view, an inevitable limitation of such a system arises from the over-reliance on the initial test scenarios that were used to design it. Even if a broad range of scenarios are used in the training phase, an extremely new scenario in the real world can throw the control system into confusion. This can lead to fatal decisions being taken. For instance, the appearance of vehicles or objects in front of the vehicle, or even the emergence of a sudden wall can cause the system to go crazy and misinterpret the prevailing ambient conditions.

### ***Deconstructing the Semi-Autonomous Vehicles***

To tackle these issues, it is absolutely important to have an underlying mathematical model that conforms to a strong theoretical basis while designing such systems. For such a model to have a precise amount of operational validity and practical performance, three important aspects have to be considered.

1. The number of components the system has to be broken into, should be optimal.
2. The model should be able to respond to difficult scenarios such as traffic congestions, steep turns, sharp curves, sudden brakes, etc.
3. The model has to be flexible enough to be extended to a plethora of automobile systems.

An important question for an engineer is to identify how many subsystems the automobile should be broken into, as a part of the modelling exercise. The number of components going into a car are numerous and one faces the challenge of being unable to clearly account for the number of components which have to be modelled. For instance, if one starts counting the number of nuts, bolts and goes into all the nitty-gritty details, it would be too much of an overkill. If one just models the system considering the big discrete entities, that might be an over-approximation as there would hardly be any subtlety in the details.

After several sessions, Dr. Bhatt and his team were able to divide the vehicle into its constituent parts namely the drivetrain, steering, suspension, torque converter, vacuum booster, brake, tyres and vehicle dynamics. The inputs which the control system can direct are the torque distribution ratio at the transmission, steering angle, torque converter clutch force and suspension height. The external disturbance though a multitude in number, are limited to rolling resistance, aerodynamic drag and gravitational pull. These are the entities which define the states of the model. The basic objective of the model is to enable safe and smooth navigation and to minimize travel time.

### ***Validating the Model***

The team has conducted several simulations to verify the reliability of the aggregated model by assuming a certain set of initial pressure conditions, flatness of the road, etc. so as to observe the trends in velocity and acceleration for a simulated ambient traffic condition. All the complicated mathematical models and convoluted differential equations come to life when the model is able to predict the vehicle behaviour for a number of test cases. In the presence of preceding vehicles, congestion, slow-moving traffic the model is able to continuously switch between braking and accelerating by skillfully altering the engine speed, throttle angle, braking force, etc.

Another oft-occurring scenario in real traffic, that of the 'Stop and Go' condition in which the vehicles stop at traffic signals without turning off the engines is also mimicked by this model which reduces the throttle input and brings the vehicle to a brief period of idleness. Thus a close resemblance of vehicle characteristics to real world behaviour is observed and hence this validates the accuracy of the model that has been developed.

The cornerstone of this model lies in the way the braking system of the vehicle has been represented. The applied braking force has to be measured with the highest possible accuracy for collision avoidance. The precision in the braking force is also an important aspect which can play a vital role in navigating through congested roads

and dangerous curves. The braking model accomplishes this by considering the mass of air in the vacuum chamber, the force applied to the vacuum booster and the master cylinder volume displacement as the important states of the system. The braking mechanism that is manifested as a result of such a theoretical modelling can achieve smooth braking rather than causing a sudden braking in the device.

### ***Pushing the frontiers of Semi-Autonomous Vehicles***

As is with any mathematical model, the applicability of it is usually confined to the system for which it has been developed. The research group has developed a model which establishes an integrated interaction amongst all the components while retaining the individuality of the components. The model is unified yet distinct, integrated yet discrete, abstract yet simple, futuristic yet relevant. The mathematical framework which has been developed can be applied to any system with a simple modification, through which the frontiers of the model can be extended to any engine, any braking mechanism and any throttle system. On a futuristic note, the model could be used to replace a particular component with something that is not existent currently and can thus predict some really innovative and intelligent subsystems within an automobile.

The larger picture in this scheme of design lies with the integration of the vehicle model with that of a large scale traffic network model. Analysis of the predictions and decisions taken by semi-autonomous vehicles operating in a given location would be instrumental in designing a traffic network that has the least possible congestion levels at all times. Efficient techniques of route planning and route allocation for the various vehicles after accounting for the geographic and environmental constraints would result in a win-win situation for all the vehicles of that location. Thus an extension from a local optimization problem for a vehicle to a global optimization problem for the traffic system as a whole can be accomplished.

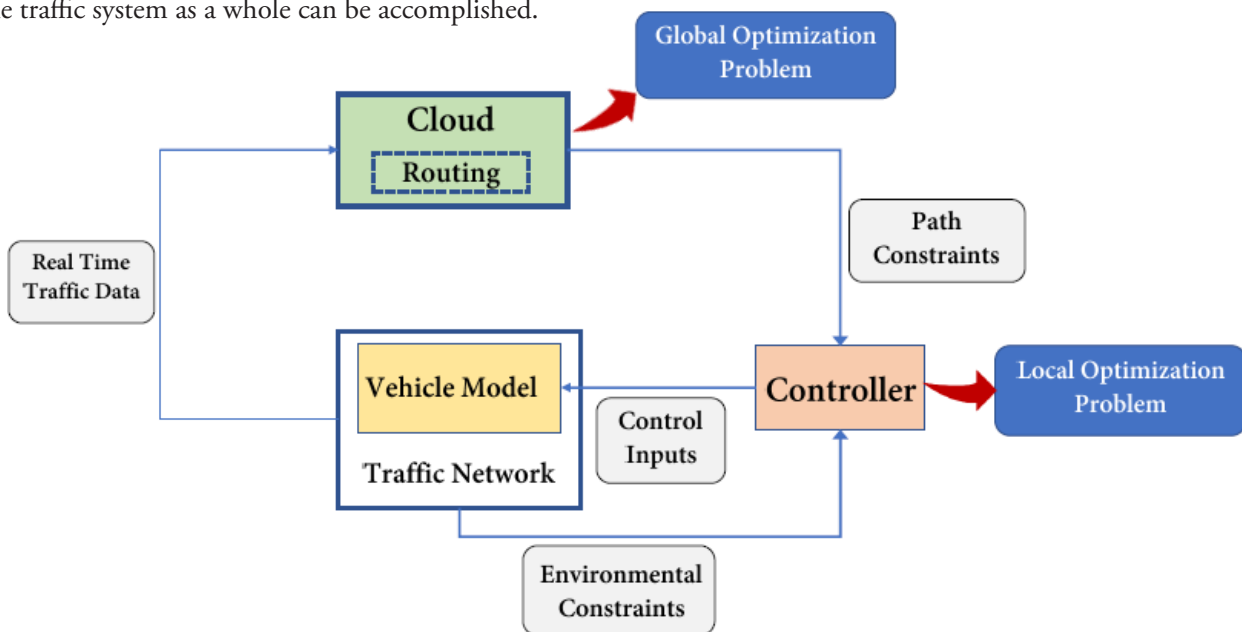


Figure : Control Architecture

The enthusiastic researcher Mr. Subhadeep's eyes gleam with perseverance and passion, and is extremely eager to explore newer frontiers of the model that has been developed. As an immediate step, strategies have been devised to accomplish the testing of the mathematical framework with a miniature table-top automobile prototype so as to add a further dimension of experimental verification to his extensive endeavours. Dr. Nirav Bhatt envisions a future, ten-years down the line when this model is industrially implemented so as to foster an era of cutting edge semi-autonomous vehicles that can make foolproof decisions in almost any real-world scenario.



**Praneeth Srivanth** (*Author*)

Praneeth is a fourth year undergrad in chemical engineering with a keen interest in anything and everything pertaining to Science and Tech. Notoriously known for being a maggu max and research enthusiast, you can occasionally hear him hum classical music tunes and play the keyboard. He loves to spend his free time being engrossed in reading musicological journals, philosophical narratives and watching vintage films.



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*Dr. Nirav Bhatt and Dr. Ramkrishna Pasumarthy with their research team*





# ELECTROCHEMISTRY

## *The Cornerstone for a Myriad of Innovations*

by Ivana Ashmita Minz

*Having found his interests roused, the professor went on to find out what the buzz was all about. What followed, was a series of innovations that even he hadn't imagined venturing into.*

*Like Newton's law is to tug-of-war and Schrodinger's equation to quantum physics, so is electrochemistry to fuel cells, solar cells, flow batteries and a lot more. 'They all belong to a common thread which is what we call electrochemistry', says Prof. Ramanujam, Associate Professor in the Dept. of Chemistry at IIT Madras.*





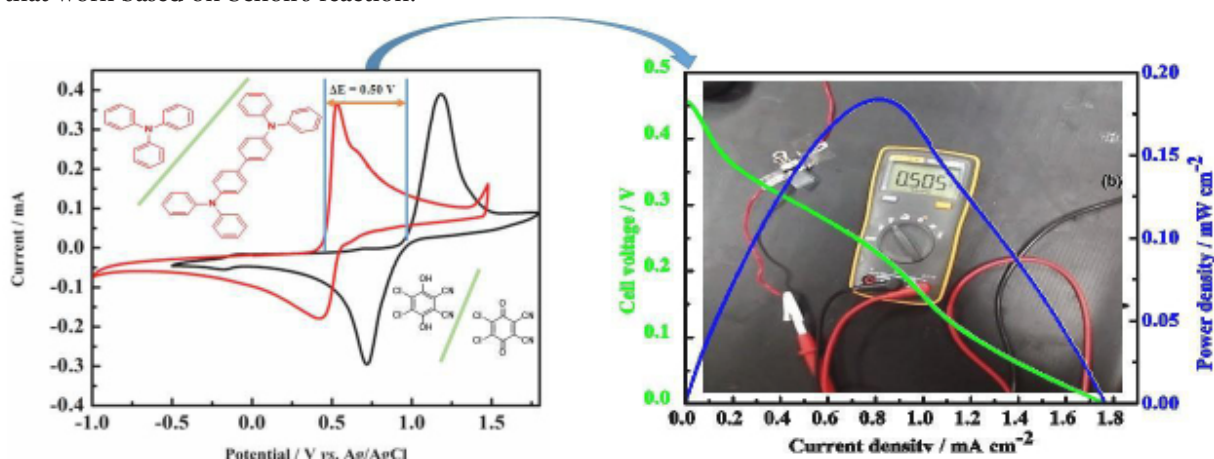
With industries setting ambitious targets to shift base of operation to renewable energy in the years to come, there is a growing demand for cutting-edge technology that will be able to deliver the best results in the field. Fuel cell technology is one such contributor to the renewable energy fix. They've been around much longer than we think. The first fuel cells were invented way back in 1838. They thrive on oxygen reduction reactions which occur under normal conditions in the presence of catalysts such as platinum. Fuel cells have been studied intensely over the years and served as the starting point of Prof. Ramanujam's research. Some of his notable accomplishments include creating a highly efficient and novel direct borohydride fuel cell (DBFC) using acidified hydrogen peroxide as oxidant and sodium borohydride in aqueous sodium hydroxide that can produce an output of up to 2V (which is well above the 1.23 V limit of aqueous system) and improving cell function of direct methanol fuel cell (DMFC) by developing cathode catalysts that are methanol-resistant, to name a few.

### Discovering New Avenues

While fuel cells may have been the professor's primary interest, new roads began opening up and he could now see newer opportunities opening in places unexpected. So, when word went around that a seminar on the construction of graphene from elemental carbon would be happening soon, the news left a bell ringing in the mind of the professor, whose work primarily revolved around fuel cells. 'What did this person's research have to do with carbon?' the professor wondered. Having found his interests roused, the professor went on to find out what the buzz was all about. What followed was a series of innovations that even he hadn't imagined venturing into.

The seminar introduced the professor to the possibility of working with what is known as Scholl's reaction. Scholl reaction is a coupling reaction between aromatic hydrocarbons in the presence of Lewis acids such as anhydrous aluminium chloride and a protic acid. The reaction has a long history, since 1910, but most applications have been during the last decade. It have been used in polymerizations, synthesis of graphene nanoribbons and various other areas. The Scholl reaction presented a fine opportunity to investigate applications of electrochemistry in the area. So, the next step was to translate this reaction into an electrochemical reaction. By conducting the oxidation of arene and reduction of 2,3-dichloro-5,6-dicyanobenzoquinone (DDQ) in separate compartments (anode and cathode), which communicate ionically through the electrolyte - methane sulphonic acid, Prof. Ramanujam and his research team were able to develop an electrochemical cell.

Following this success, present efforts of research scholars in this area are directed towards developing small cells that work based on Scholl's reaction.



Experimental Results & Setup of the Scholl Reaction Based Electrochemical Cell.

### Organic Molecules – A Renewable Alternative

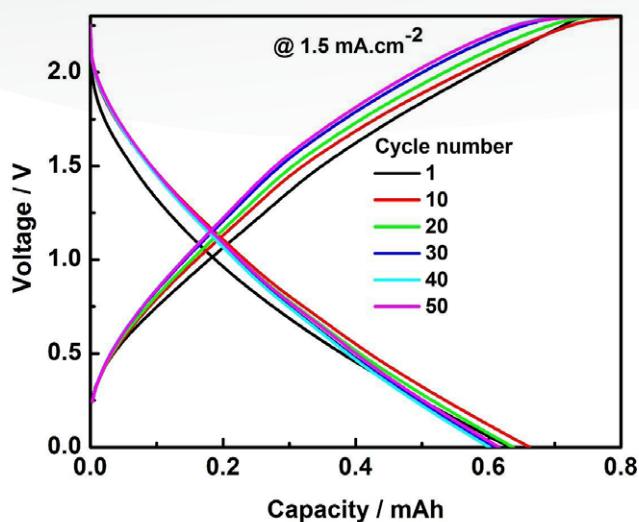
Another technology that Prof. Ramanujam's team has been toying around with, is the use of organic molecules in making replacements for the components that go into making a cell.

In the push towards utilizing renewable energy sources to meet energy demands, there is a need for better performing batteries. Batteries play a crucial role in the energy storage requirements of energy captured by solar



cells, wind turbines and the like. Traditional batteries for this purpose have turned out to be either inefficient, or too expensive. It is therefore essential to develop batteries of economic value performing at par with these traditional batteries that can serve as a good fit for the renewable energy harvesting stations.

Unlike conventional batteries and fuel cells which require platinum and electrodes made of transient metals and lithium, which can be quite cost-intensive and where sourcing the metals may prove to be a difficulty, a ready solution lies in making use of organic molecules and developing complexes that can go into batteries and replace the metals. These new substitutes are a renewable alternative and cheaper too.



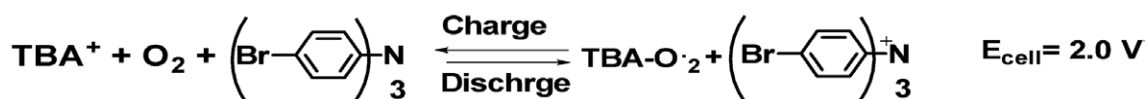
Charge/Discharge cycles of the Organic Battery

Flow batteries bear much resemblance in infrastructure with fuel cells. They consist of an electrochemical conversion hardware and chemical storage tanks. The energy storage is limited only by the size of these tanks.

Prof. Ramanujam and his students, along with Prof. S. Sankaraman have designed redox couples that can go into these organic redox flow batteries. By doing so, they have been able to achieve an output of up to 2V per cell that can be run in over 200 cycles and still give the same power.

Probing further, Prof. Ramanujam says that the entry into this field was in many ways serendipity. With the initial goal being to study the redox property of a material called

tetrabutylammoniumhexafluorophosphate (TBAP), to their surprise, the professor and his team landed with some unusual results. Re-examining the whole procedure, it was found that a student had forgotten to deoxygenate the



The net reaction occurring in the battery.

medium. Lucky for them, this turned out to be a means to discovering a new redox couple altogether! They found that in the presence of TBAP as electrolyte, oxygen when present, undergoes a redox reaction to form super oxides. The product of this reaction (superoxide) which is otherwise unstable, becomes stable in the presence of TBAP cations. Then, using 4-bromotriphenylamine to make another redox couple and combining it with the setup above, the team was able to assemble a cell that gave an voltage output of up to 2V.

The performance was evaluated to be stable with the advantage resting in the fact that the cell inputs such as the membrane and electrodes were reasonably cheap and can be manufactured within India, thus eliminating the need for overhead expenditures in import of metals.

### A Second Serendipity

What if you had the power to exercise control over the lifetime of a battery? That, until necessary, you could keep it in its dry state (i.e. without the electrolyte) and get it into action only when time called for it? This could mean a great deal to armies on the frontlines who require reliable and large amounts of energy sources for a variety of purposes. So that when the time calls for war, these devices could be deployed without delay and also without fear of the system failing to deliver reliable power.

It may seem hard to imagine, but Prof. Ramanujam's research group has figured out a means to realize this idea. This is where we begin to look beyond primary and secondary batteries to reserve batteries.

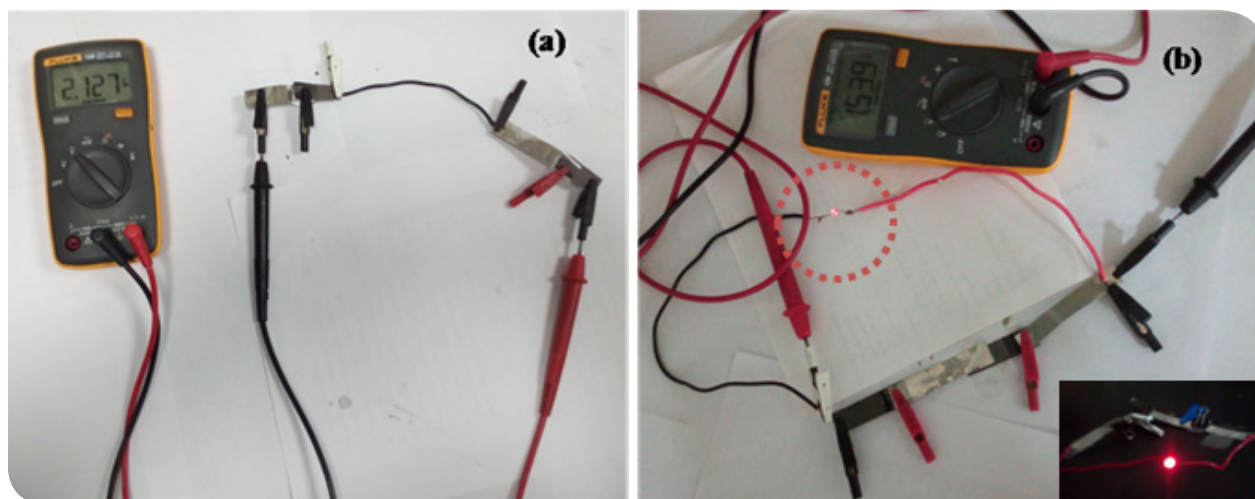




The fact that iron oxidizes vigorously with hydrogen evolution in an acidic medium isn't too alien a fact for many of us. Also, batteries have been developed with iron in alkaline media consisting of metals such as nickel or cadmium in the cathode. But what if we tweaked the conditions such that iron in acidic medium did become a source of harnessing power? The professor calls this discovery another serendipity.

The system under study consisted of stainless steel which was being used to oxidize triphenylamine in an acidic medium consisting of methane sulphonic acid. It was found that even in the absence of triphenylamine, the stainless steel & methane sulphonic acid combination showed an oxidation peak. Further study revealed that it was stainless steel which was undergoing oxidation in the system. Unlike pure iron itself, stainless steel doesn't undergo corrosion that readily and its oxidation is a relatively controlled reaction. When combined with an oxidant such as dichlorodicyanobenzoquinone (DDQ), an organic substance, we have yet another battery.

The Fe-DDQ couple forms a reserve battery which remains inactive until the addition of methane sulphonic acid. This battery is able to raise the voltage to upto 1 V. Two cells in series powering RED LED is shown below, wherein stainless steel act as a Fe source and DDQ as cathode.



*Cell voltage of two cells in series*

*Two cells stack powering LED*

This discovery is yet another addition to the list of innovations contributing to the renewable energy cause from Prof. Ramanujam's lab.

### ***Chemistry of Dyes & Solar Cells***

In another episode of adventures, this time tapping on their strength as students of Chemistry and their deep-well of knowledge about the synthesis of complex molecules, in collaboration with Prof. Indrapal Singh Aidhen and Prof. R Dhamodharan, who also belong to the Dept. of Chemistry at IIT Madras, Prof. Ramanujam and his team worked together to produce a new dye consisting of phenothiazine conjugated to an ethynyl-pyrene moiety.

A typical dye sensitive solar cell consists of a semiconductor such as titanium dioxide (TiO<sub>2</sub>) to separate holes from the electrons and it serves as a roadway for electrons coursing through the cell. The TiO<sub>2</sub> particles are coated with a sensitizer which is an organic dye that may be a metal containing dye or a metal-free dye. The sensitizer injects electrons into the conduction bands of semiconductor upon absorption of photons that come from a light source. The cell also consists of a liquid electrolyte composed of iodide which replenishes the electrons leaving the dye. Platinum is used as the counter electrode and dye-coated TiO<sub>2</sub> as the working electrode. With the use of the newly produced dye, the team was able to achieve up to 12% photoconversion efficiency, patently making it one of the best dyes in literature for dye sensitive solar cells as of now. So we see that dyes play a crucial role in the working of solar cells. Though at first it may seem strangely disconnected to us, the applications and benefits are plenty!

Additionally, one can introduce several other modifications into the system to improve its functioning, such as changing the electrolyte so that the dye can perform optimally or even changing the structure of the dye itself. In fact, quantum-mechanical modeling of the system help identify features of the dye that make it suitable for dye sensitive solar cell applications. This information can later be used as a database to refer against and make further advancements in the field. Clearly, the field of renewable energy combined with chemistry is vast and wide open, encouraging curious minds to push the boundaries of innovation and bring about the next breakthrough.

### **Looking Ahead**

The effort towards developing these technologies is not singular. It calls for collaboration across several departments and simultaneously, reinforcing relationships with industries which seek to incorporate this technology into their businesses. One of the recent initiatives undertaken at IIT Madras, is the creation of a 'solar hub', officially named as the Indian Solar Energy Harnessing Center (ISEHC) which will see the participation of students and professors from various departments across the campus with the singular goal of making these revolutionary technologies a reality for the nation.

*'Electrochemical energy storage and photovoltaic solar cells are going to be the next big things from IIT Madras within the next decade'*, exclaims Prof. Ramanujam in a quiet tone of confidence. He believes, along with the wider research community at IIT Madras, that the fruits of success that await to be touched upon are just around the corner.



#### **Ivana Ashmita Minz (Author)**

Ivana is a third year undergraduate in the Chemical Engineering Dept. As a curious bug, she is one who asks the- What? Why? & How? -of just about everything. One can find her head stuck between the pages of a book, probably seeking answers to one of the several questions she carries in her mind. She uses writing as a means to articulate her thoughts and has certainly found a means to 'IMMERSE' herself in it!



**Dr. Kothandaraman Ramanujam** is an Assistant Professor in the Chemistry Department at IIT Madras. He is a Gold medallist in B.Sc (Chemistry) which he obtained at Sri Vasavi College, Affiliated to Bharatiyar University, Coimbatore in 1998. Following this, he completed M.Sc (Applied Chemistry) from Anna University, Chennai in 2000 and was then awarded a PhD from the Indian Institute of Science, Bangalore in 2006. He specializes in Electrochemical Systems (Fuel Cells, Batteries and Organic Solar Cells) and is an active reviewer of Journal of the Electrochemical Society, International Journal of Hydrogen Energy, and Bulletin of Materials Sciences, Journal of Chemical Sciences.



*Dr. Kothandaraman Ramanujam and his research group*





## *WHEN MR. VEHICLE SAVES THE DAY (AND NIGHT)*

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*by Akhil Sathuluri*

*Driving can be fun, but for most of us, it is an indispensable activity in our day to day lives. We travel from place to place to get things done and meet new people. Driving in India is a unique experience owing to the variety in traffic composition and volume. But, from the perspective of daily drivers of buses, trucks, lorries and tractors, this can make driving a nightmare. Driving, in this case, is a responsibility which demands a lot of caution and safety, for there are expectations involved. Given this, Prof. Shankar Ram and his research scholars are all set to answer how the freedom and fun of driving can be restored. They are excited to be developing systems that enable the vehicle to make its own decisions when the driver cannot, especially when there is an emergency. When devised right, they just work when needed, like magic!*





### The Indian Scenario

Indian traffic is heterogeneous. There are vehicles from across the spectrum including two-wheelers, bikes, cars, tempo travellers, lorries, light commercial vehicles and auto rickshaws, to name a few, all constituting it. Diving into some statistics reflects a few important facts. Nearly 5-6% of the heavy vehicle population in India (which includes buses, trucks, and tractors) account for close to 30% of the road accident fatalities. This large number can be attributed to the high fatality rate that is associated with an accident involving a heavy vehicle. The next issue is that, in order to save time, for last-minute convenience or due to berth shortages in other modes of travel such as trains, a significant number of people prefer overnight travel by buses. Night travel is always risky and we would need advanced control systems to augment the safety of the passengers. On the other hand, most often, simple passive measures by the drivers can avert fatal accidents. Consider the act of switching on of hazard lights while changing a flat tyre of your car; this would not be of much concern in broad daylight, but for a bus coming at 100 km/h at night, this would mean life or death as the driver would not have much time to react only once he/she sees the car. Maintenance is something that can be easily taken care of, despite that we see accidents due to ill-maintained vehicles. So, designing of good vehicles is only part of the solution, and the vehicles have to be maintained properly. For example, according to the Indian automotive laws, there are very strict standards with regard to automotive braking that are well followed by vehicle manufacturers. Frequent maintenance inspections are necessary to prevent any major problem during a vehicle's operational time. But a fleet operator who runs several hundreds of trucks daily might not pay much attention to this. Hence, enforcement inspections by traffic police should also happen from time to time. Despite strict and unique Indian laws like a mandatory Anti-lock Braking System (ABS), which prevents uncontrolled skidding of the wheels during braking, for all heavy road vehicles, we see a lot of fatalities every year. All of these are a few operational issues in India. For example, Figure 1 shows the result of a Hardware-in-Loop (HiL) simulation of a vehicle with well-maintained brakes and a vehicle with defective brakes. One can observe the change in orientation with a defective brake.

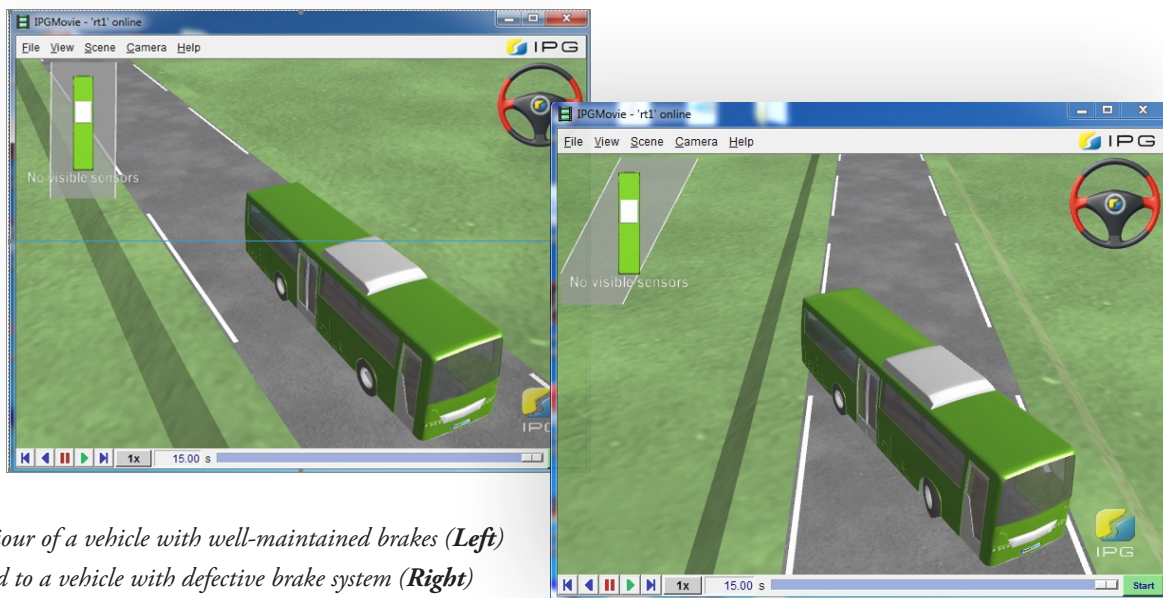


Fig. 1:  
Behaviour of a vehicle with well-maintained brakes (**Left**)  
opposed to a vehicle with defective brake system (**Right**)

The problem can, therefore, be broken into two: better vehicle design, where the vehicles are upgraded to higher safety standards and pack “smart” systems to assist the driver, and better driving atmosphere, which involves improvement of the factors that influence driving. However, the latter is a bigger challenge which lies in the hands of the public and policymakers. The heterogeneous traffic of India means that the same safety strategy cannot be applicable in all scenarios. This is strikingly in contrast with the western world, which has a fairly homogenous traffic. As a result of the heterogeneity, we are usually surrounded by various kinds of vehicles during our travel. In such an environment, it is important to note that different vehicles have different braking characteristics and different response times to stop during an emergency. This means each class of vehicle has a varying time to accelerate to a required speed or decelerate to a halt. This makes the problem much more challenging.



Thus, the research group from the Automotive Control Laboratory at the Department of Engineering Design has been working on solutions for these problems keeping in mind the ground reality in India. They develop systems that assist drivers to take better decisions. Their aim is to design a comprehensive system that is capable of diagnosing critical braking parameters and monitoring of the braking components while at the same time, being retrofittable and affordable. This makes it easy for the users to add them to the dashboard without having to buy a whole new vehicle! It should be capable of cautioning not only the driver but also the owner and concerned authority who can be connected in the loop at a time of need. This connected driving system can be used to communicate the necessary corrective action to the driver. The safety of the vehicle can also be monitored via a smartphone or any such connected device. This temporal data and record of information can be shared and analysed for meaningful insights which may help the owner to predict vehicle maintenance dates and component replacements.

### ***Designing the System***

Heavy vehicles differ drastically from passenger cars with respect to weight, load carrying capacity and speed limits. Consider a scenario where a load is carried by a 12 tonne truck in its fully laden state. As the load is dropped off at its destination, there will be a huge change in the mass of the vehicle (up to 4 tonne). The engine and brakes of a heavy vehicle are designed to deliver the required performance under fully laden conditions. So, in the unladen condition, such specifications would be an overkill and may lead to instabilities in a maneuver. In contrast to a heavy vehicle, a passenger car has lower changes in its mass. Also, a heavy vehicle has its center of mass at a considerably higher position compared with a passenger car, leading to coupled problems in vehicle dynamics. While analyzing a passenger car, one may consider effects of longitudinal, lateral and the vertical motions separately, but one might fall in trouble if the same thing is assumed for a heavy vehicle. From the scientific point of view, these problems become challenging. George Westinghouse invented air brake systems in the early 1880s. Since then, they have been used widely in heavy road vehicles. The response times of air brakes are much higher than the response times of conventional hydraulic brakes used in passenger cars. The response time is an important parameter that affects the vehicle stopping distance and influences the time available for corrective action during an impending collision. Though there has been a significant improvement in the technology as such, the fundamental working methodology has remained the same.

The professor and his group have developed a collision avoidance system. As the name suggests, this warns the driver if the vehicle is in danger of an impending collision. For a driver who drives long distances, physical and cognitive fatigue are important issues to be addressed. Drowsiness affects the concentration of the driver and this may lead to collisions. Vehicles having a collision warning/avoidance system alert the driver under such conditions and can also take over the control of the vehicle if any responsive corrective action is not taken. “Adaptation and acceptance are the key challenges of such a technology”, Dr. Shankar Ram says. The assistance by these systems should not be too intrusive and at the same time, should be catering to the specific user set. Despite having all the advanced sensors, actuators and controllers in the vehicle, the important thing is that the driver should feel comfortable with them because he/she is the one who is going to interact with this technology on a day to day basis. An unnecessary intervention may perturb the driver, making him/her disable the entire system, defeating its purpose.

The research group is working on developing dynamic system controllers and are tuning them for different scenarios, incorporating all the aspects of a typical Indian traffic setting. So, a system running solely with a collision warning system where a driver is responsible for corrective action would stand ineffective if no action is actually taken. How useful is it to detect a collision when the driver is not in a state to avoid it? The idea is to give some level of autonomy to the vehicle to take corrective action on its own itself when the driver is not in a state to respond. Here, a collision avoidance system along with a collision warning system will automatically take control over the system if the driver does not take any corrective action to prevent the impending collision. This is important while on a bus traveling at high speeds at night, with a possibly drowsy driver, who is not paying attention to obstacles

in the course, manning it. This situation is more probable today with vehicles running at very higher speeds on our highways. Buses of yesteryears traveled at 40-60 km/h but now they travel at nearly 100 km/h on the same roads, raising questions of safety.

### *Validation of the Developed Systems*

A proof of the concept is as important as formulation, and analysis and validation are important before deploying into real systems. It is not enough to implement these ideas via computer simulations when people's lives are at stake. The derived model parameters of the test vehicle should ideally be tested by running it on a test track. However, it is very difficult to evaluate a developing technology on a real test track multiple times as there is always a high factor of risk associated with this process.

A completely custom-designed Hardware-in-Loop (HiL) heavy vehicle test facility has been set up in the Department of Engineering Design for this purpose. Figure 2 shows the setup which consists of a physical brake system setting of a heavy vehicle along with controllers and the software counterparts. It helps transfer data between the physical system and the virtual model developed and enables the user to visualise the effect of the controller in real time. With the help of a commercially available software called IPG TruckMaker, the whole heavy vehicle

simulation can be done by interfacing the software and hardware to capture the system's response. Such testing would bring down the risk and instill confidence before deployment.

The IPG TruckMaker software enables one to create and evaluate mathematical models through computer simulation. In this case, these simulations are augmented by the HiL testing facility. Models and variables for all the subsystems can be manually selected. Flexibility in the environment type, engine type and other such parameters are used to simulate various situations. These simulations give us an understanding of the effects on the vehicle under these multiple scenarios and parameters. Virtual sensors used in the software provide us processed data and a real-time visualisation of what is happening. These datasets from the hardware can later be post-processed, say by using a MATLAB script, to weigh it against the simulated (hardware-in-loop) virtual (software) model. This comparison is used for validation of the models. Improvements are then made by incorporating more terms to increase the accuracy of the result. These developed controllers are then used to find the different physical parameters



*Fig. 2: Hardware-in-loop testing facility of a heavy vehicle*

corresponding to the vehicle which may help in the design phase. Various practical road conditions, like wet and dry surfaces, leading to potential wheel 'locking' and vehicle instability are also simulated. Generally, the hardware cannot keep up with the computational speed of the controller, leading to a mismatch between the action taken by the driver and the output at the wheels where braking actually happens. This can be attributed to the response time of the mechanism providing the braking action. For example, though we press the brake immediately after seeing an obstacle on the path, the brake chamber pressure cannot increase instantaneously for the opening or closing of the brake valves. This problem has to be dealt with first and a separate control algorithm handles this problem. The experimental setup shown in Figure 2 is built with an electro-pneumatic actuator for faster response times than the





*Fig. 3: Simulation of a virtual truck mode*

strategies for each of them. This research paves the path to many intelligent descendants of the current version of automobiles. Their higher autonomy would assist the drivers to take decisions much faster and effectively. Let us hope this harmony between man and machine would reduce the number of road accident fatalities in the future.

The research group is working on developing dynamic system controllers and are tuning them for different scenarios, incorporating all the aspects of a typical Indian traffic setting. So, a system running solely with a collision warning system where a driver is responsible for corrective action would stand ineffective if no action is actually taken. How useful is it to detect a collision when the driver is not in a state to avoid it? The idea is to give some level of autonomy to the vehicle to take corrective action on its own itself when the driver is not in a state to respond. Here, a collision avoidance system along with a collision warning system will automatically take control over the system if the driver does not take any corrective action to prevent the impending collision. This is important while on a bus traveling at high speeds at night, with a possibly drowsy driver, who is not paying attention to obstacles in the course, manning it. This situation is more probable today with vehicles running at very higher speeds on our highways. Buses of yesteryears traveled at 40-60 km/h but now they travel at nearly 100 km/h on the same roads, raising questions of safety.



*The Automotive Control Lab Research Group along with Dr. Shankar Ram.*



**Akhil Sathuluri (Author)**

Akhil can be found thinking about the next big upgrade to the imaginary robot he has never built. His interests keep changing with the seasons and currently wants to become an expert cook. He never says no to the one last round of online gaming. He's a fourth year undergraduate from the Department of Engineering Design with his interest peaking at robotics and control and the rest distributed uniformly on anything from origami to graphic design. He wishes to complete building his robot one day.



**Dr. C. S. Shankar Ram** is currently an Associate Professor at the Department of Engineering Design, IIT Madras, since joining it as an Assistant Professor in 2006. He was awarded a Ph.D. from the Texas A&M University. His research interests include the fields of Dynamic Model-Based Analysis and Control of Vehicle Systems, Advanced Driver Assistive Systems and Hybrid and Electric Vehicles. He has also been working on transportation systems including traffic flow modeling and control.





## The Less Stiff the Better

by Ramya Kannan & Sruthi Guru

*For the past few decades, lifestyle changes, including an increase in the consumption of fast food, have increased the risk factors for cardiovascular diseases (CVDs). Current research on early detection and diagnosis of CVDs has opened up new avenues in clinical diagnostics, whose findings can help us in early diagnosis and modifying our style of living. The use of non-invasive techniques using ultrasound has become a new scientific tool being researched at Department of Electrical Engineering, IIT Madras in the group led by Dr. Mohanasankar Sivaprakasam.*





Cardiology as a whole encompasses information about the heart - the vascular system, blood vessels, lifestyle and patient history, which make the heart one of the most complicated systems to study and monitor. Cardiovascular diseases include different conditions relating to the improper functioning of the heart and but they are mostly associated with atherosclerosis (a disease of the arteries characterized by the deposition of fatty material or plaque on their inner walls). There are two types of heart attacks — cardiac arrest, which happens when the heart fails, and a systemic attack which involves blocks in the coronary artery. Prior to the systemic attack, there are many progressive stages, which may be due to a muscular injury or plaque deposition, leading to a possibility of diagnosis. The stiffening of arteries happens in a very early phase of cardiovascular disease progression. Though arterial stiffness increases with aging and various disease states, there is an increasing evidence of the stiffness of arterial wall in subjects with high risk factors for CVD event. Increased arterial stiffness is an indicator of vascular injury and an early indicator of future cardiovascular events. Moreover, as vascular stiffness is a modifiable risk factor, which can be controlled by exercise, diet and health-lifestyle choices as well as by medication, which makes it very significant in early detection and prevention. However, detection of stiffness is useful as early detection could help modify lifestyle to prevent disease onset. The requirement for a device with a non-invasive technique which could measure arterial wall thickness as an indication of the onset of cardiovascular disease was thought of as a PhD problem way back in 2007, at the Department of Electrical Engineering, IIT Madras. Today, at the same department, Dr. Mohanasankar Sivaprakasam and his team, have focused on translating this technology from a laboratory to a device, through the activities of HTIC (Healthcare Technology and Innovation Centre), a joint initiative of IIT Madras and Department of Biotechnology, Ministry of Science and Technology, centered at IIT Madras Research Park. He is the Director of HTIC.

The myriad possibilities of basic science research, translating into a technology has always been intriguing and this translational research is popularly known as “bench to bedside”. Being a translational scientist himself, Dr. Jayaraj Joseph, Chief Technologist of HTIC and an IITM alumnus, was the brain behind developing a non-invasive device to measure arterial wall stiffness during his PhD. He walks us through the HTIC at IITM Research Park for a detailed discussion on this translational research at their laboratory. With a strong vision of thinking about the impact of our research on society and its usability in the actual field before embarking on any project, he makes it very clear that research over the years has grown from being a laboratory scale product development to a product evaluation based on exhaustive field studies. This could also lead to product deployment on a commercial scale. HTIC, being a research and development based centre, works closely with industries in developing R&D solutions and joint development of technology products and technology assessment in the healthcare sector.

“A translational scientist should be able to move an idea all the way from basic research to a clinical application and back to the lab to inform basic science”

*Mary Druss, Oncologist, Univ of Washington*

The current technology widely used to monitor arterial wall thickness is an imaging-based technology which is expensive, requires a trained operator, and could not be used to measure arterial wall stiffness on a large scale for a strained population due to the Pre-Conception and Pre-Natal Diagnostic Techniques (PCNDT) Act, 2003 in India, which has severe restriction on the utility of ultrasound imaging in clinics and hospitals across India. Hence, to overcome these drawbacks, the team had to come up with a new system which could identify the artery, study their movements and measure the stiffness; all these without any visual observation! They devised a non-invasive ultrasound-based method to detect the echoes from the artery upon sending ultrasound pulses to measure the arterial wall stiffness. The work initially began in an environment where the concept of image-free recordings was gaining importance. One of the bottlenecks while developing algorithms was that unlike in the case of common cardiograms (like ECG, EEG, etc.) where there are many online databases, ultrasonic sound signals did not have a good online database. The origin of this product development began in the Non-Destructive Testing (NDT) lab of Department of Mechanical Engineering, IITM. The first experiments to explore looking into the artery using a single ultrasound transducer were done in the NDT lab. Following encouraging results, a dedicated experimental



hardware setup was developed in Department of Electrical Engg, IIT Madras for extended testing and research. It is important to note that when one sends a sound signal, a lot many echo signals are produced from the complicated human anatomy, which contains artery, vein and lot of muscles. So, one has to figure out which is the echo signal characteristic of the artery, and also how to identify the carotid artery. Based on well-known anatomical findings, it was assumed that the strongest moving structure is the artery, amongst others, the motion being predominant.

The device has a transducer, which converts vibrations into sound signals, which was custom-designed with specific focal length and narrow beam width to make it highly directional.

Thus, when it is placed perpendicular to the wall, strong spectra of reflections are obtained from the arterial walls along the diameter of the artery. The rough location of an artery can be deduced from the known anatomy of the heart. The range and depth of echo signals are also measured as the arteries are actually moving with nearer and farther (proximal and distal) walls moving in different directions. Considering this movement, multipurpose algorithms were developed which perform arterial wall movement based on multiple features, mainly wall motion and its impact on echo signal. At that time, it was a tough call as no image was available, one had to internalize the features of the echo, amplitude and characteristic motion. Once the basic algorithm was developed, it had to be tested for any weaknesses and improved upon. During his Ph.D., Dr. Joseph performed experimental simulations and developed phantom algorithms which were tested on very limited human subjects. This was done mainly to demonstrate that a fully functional system, which was not perfect, was able to measure the dimensions of an artery.

$$\text{Elastic modulus } (E_p) = (\Delta P \times D_d) / \Delta D$$

$$\text{Stiffness index } (\beta) = \frac{\ln(P_s/P_d)}{(\Delta D)/D_d}$$

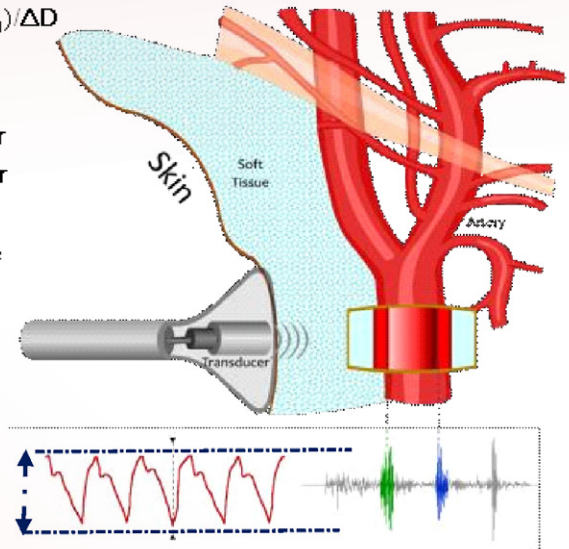
$D_s$  = Maximum systolic diameter

$D_d$  = Minimum diastolic diameter

$P_s$  = Maximum systolic pressure

$P_d$  = Minimum diastolic pressure

$$\Delta D = D_s - D_d, \Delta P = P_s - P_d$$



*Ultrasound echo signal of the arterial wall*

Arterial stiffness (AS) is said to be an important marker in early stages of cardiovascular diseases, out of which local arterial stiffness (LAS) and regional arterial stiffness (RAS) are two major measurement techniques. LAS is evaluated based on measuring the contraction/expansion of arterial wall (also called distension) and lumen diameter (the difference between proximal and distal walls) of the carotid artery as delta d. RAS is generally obtained by evaluating carotid to femoral pulse wave velocity (cfPWV) through tonometric devices. RAS has a better prognostic value than LAS and cfPWV is considered as the gold standard of AS. Unlike in images where you can estimate the dimensions, the ultrasonic sound echoes are not images, they are a representation of the physical structure in the form of sound. Depending on the material and the designed transducer, one would observe reflections unlike the ones coming from a sharp edge. Thus, one needs different types of algorithms to model the ultrasound signal, the entire range of variations, etc., in order to find the where the exact boundary is for measuring the inner diameter of the artery. As a result, two algorithms were developed — one that processes the motion as to how much the artery expands and contracts, which is called distension; and another set of algorithms used to measure the inner lumen diameter. The latter needed a second algorithm due to the technical challenges in accurately measuring the inner diameter of the artery. On moving from inside out, one can see a nice strong echo, but while one echo would be strong, the other echoes would be dispersed; therefore, several iterations for improving the signal-to-noise ratio were performed and the algorithms were scrutinized. Improving upon this experimental setup, a basic functional hardware was developed in form of a desktop prototype. This entails a typical Ph.D. problem – develop hardware, make as many people as possible to collaborate with you, and so on. Then the problem moved from academia to industry when HTIC was set up, and the project resumed in 2011. The technology was then termed as ARTSENS



*ARTSENS measures carotid artery stiffness of a volunteer*

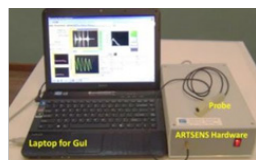
(ARTerial Stiffness Evaluation for Non-invasive Screening). A lot of feature-based algorithms were developed which looked at the various features of the echo signals coming from the artery.

Now, the challenge was how to translate ARTSENS to the real world. A gap which comes in the development of new technologies in any laboratory is lack of enough validation in the field, limited usability, and practicability of the developed products. Translation includes validation of the product in the field at multiple places.

The thought process undergoes a change when one works in a lab and when one wants the product to go into the field. This is because in the laboratory if the concerned person is available, the product will make progress; however, in HTIC all the products are developed by teams. For ARTSENS, before taking the product to the field, some level of translational engineering was done that included improving the usability, reliability and making it amenable to field employment.

A major challenge was encountered by the team during one of the field studies done within four to five months of the project being taken up by HTIC in 2011, where the first desktop prototype was first tested in Mediscan Systems, Chennai. This field study included 106 subjects, and during this study it was found that the product worked perfectly when the subject was in sitting posture, generating strong echo signal characteristic of the carotid artery. However, when the subject was in lying position, the jugular vein, which is placed right next to the carotid artery was pulsing, and the algorithm was unable to differentiate whether the echo signal was coming from the jugular vein or the carotid artery. So, over the next three to four days, the team was continuously accelerating the technology development with multiple iterations to improve usability based on integrated feedback. This experience taught the importance of field study and how it enriches research; simulation in the lab has its own limitations, therefore, HTIC exposes students to field work as much as possible. Due to the students working on the project, noticeable acceleration in product development was observed. One of the Ph.D. scholars involved was Mr. Ashish, who works on improving algorithms for entire ARTSENS for distension, diameter measurement, and jugular vein projection. Some students work on hardware development and improvement for miniaturization of electronics involving embedded systems development. Mr. Preejith, an MS scholar of Dept of EE was instrumental in developing the first portable version of ARTSENS using custom embedded systems hardware. The team has come a long way in developing hardware prototype from a functional desktop prototype to ARTSENS Pen (2015) and ARTSENS Touch (2016) developed recently.

A point of observation during this gradation of hardware development is that every time one changes some component, one has to validate the hardware through testing and simultaneously also improve the algorithms based on feedback as a part of quality measures. The device is first placed on the neck of the patient, then after identifying the artery, it is probed by getting angulated by the device



**ARTSENS Desktop (2011)**



**ARTSENS Touch (2013)**



**ARTSENS Portable (2014)**



**ARTSENS Touch v2 (2014)**



**ARTSENS Mobile**



**ARTSENS Pen (2016)**

(computing the position based on angle measurements) and within 30 seconds the signal is obtained. In practical usage, tentatively the devices take 5 to 10 minutes for recording if one finds the artery; it takes more time for a difficult segment. Further, signal quality conditions also need to be considered. A series of very effective signal quality conditions were developed by Mr. Malay Shah, one of our MS Scholars, who subsequently also was part of the technology development & clinical validation of ARTSENS. Hence, the recorder could reject poor quality signals, crack the signal, obtain waveforms, pick the right waveform, average it and give the correct waveform. Once an algorithm was developed which could identify and reject echoes from the jugular vein, different field studies helped in iterations for the validation of both the hardware and the algorithm. The ARTSENS device was also compared with existing devices that could measure RAS and was found to be highly competitive with accurate values for the lumen diameter. The ARTSENS probe was successfully strengthened by its fine placement of probe, arterial wall tracking method, a well- distinguished algorithm to differentiate an artery from a vein, and also the measurement of the pulse wave velocity, a gold standard for stiffness measure.

Recently, another study was carried out by ICMR-National Institute of Epidemiology (NIE), Chennai, tested over 1000 subjects, where the personnel using the equipment were not trained medical practitioners but were specialists who study health and disease conditions. The current success of the product can be measured in terms of translating it from laboratory to the field by testing it on more than 3000 subjects. Further, the product is being validated in many international centers as well so that the testing of subjects closes upon a 10000 mark. For



*Dr. Jayaraj Joseph demonstrating ARTSENS live on stage at NI Week 2015 in Austin, Texas*

any product, commercial success cannot be done without validation in large numbers as well as multiple places. Thus, the focus has now shifted to validation dynamics. Device usability in the field was tested by NIE field study, while the utility of the device in the screening of diagnosis is being tested in collaboration with various centers like Thambiran Heart & Vascular Institute and Sri Ramachandra University, Chennai. The takeaway point from the field studies helped them in making the device more amenable and user-friendly, with miniaturization of the hardware. Using this criterion, another device 'ARTSENS Mobile' was developed in collaboration with National Instruments. ARTSENS Mobile was first displayed in a premier event organized by National Instruments in Austin, Texas as a part of their annually held event, and was selected as the best customer application of the year 2015! Further miniaturization was achieved in form of ARTSENS Pen which was developed in 2015 and was validated on more than 550 subjects this year at Voluntary Health Services Hospital, Chennai. An extensive set of clinical validation studies is also being planned.

Using this core technology for spurring the next set of major research works, the relentless team continues on its pursuit of enhancing the product's features by not limiting it to be only an early stage screening device where the actual screening efficiency may not be that high. The future research plans of the team are to integrate ARTSENS with another device to measure some more parameters. However, the challenge with measuring multiple elements and features is their interaction among each other, and the challenge in optimising the device to perform efficiently. The team is also exploring the prospect of applying ARTSENS for measuring blood pressure and vascular stiffness, thereby increasing its clinical usability in such a manner that practically, a cardiologist will find a good use for it. One advantage of measuring vascular thickness is that it being modifiable through physical activity and exercises, this device can give a warning in advance and help the patient take preventive measures





*Validation studies of ARTSENS device in the field*

before the onset of the disease. Measuring blood pressure without using calibration is still a challenging problem in the industry. The team, including two Ph.D. scholars, has taken up this challenge and using the funding grant provided by DST and NIH propose to promote ARTSENS as a single device that can measure multiple useful parameters including blood pressure and arterial stiffness. The idea of commercializing the product as a blood pressure measuring device rather than just a screening device makes it more useful.

“Research has always been the prime focus of our institute, with research primarily concerning laboratory-scale research. Only when conversing with experts who have travelled the difficult path from academia to industry do we get to know the different aspects of research, namely, basic research and applied research”, says Dr. Joseph, who concludes with a strong message for students that impact on healthcare can be made through field studies involving clinical research and strong validation. The biggest challenge lies in getting clinicians interested and making engineers understand usability and the practical challenges in the field.



**Ramya Kannan** (*Author*)

Ramya Kannan is an interdisciplinary research scholar from the Department of Chemistry and Biotechnology working with dendrimers for biomedical applications. Apart from running between the two labs, She can be mostly found reading (fiction/ popular science) with some loud music plugged in.

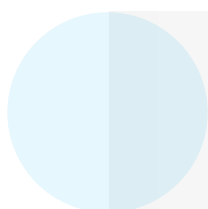


**Sruthi Guru** (*Author*)

Sruthi Guru is a research scholar in the Department of Chemistry, working in the area of materials chemistry. She loves to fool around in the lab, play with chemicals to synthesize novel materials having new properties and useful applications in the field of catalysis. Main inspiration for taking up research were the Honey, I shrunk the kids, type of sci-fi movies. Now, she is shrinking materials to nanoscale levels and hopes to strike gold sometime soon. Apart from research, she likes to draw inspiration from



**Dr. Mohanasankar Sivaprakasam** is an Associate Professor in the Department of Electrical Engineering and Director of HTIC, IITM Research Park. His major goal of developing affordable medical technologies in the country is being successfully accomplished by his brainchild HTIC, which is an ecosystem of technologists, clinicians and industry.



**Dr. Jayaraj Joseph** is the Chief Technologist of HTIC and an IIT Madras Alumnus, and he works on hardware projects involving sensors and instrumentation, system integration and medical device development. His main research interests apart from biomedical instrumentation include automated test and measurement, virtual instrumentation, and renewable energy resources.

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# The Migration Migrane

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by Venkataraman Ganesh

*The 1991 liberalization of the Indian economy has unleashed a wave of migration within India. This has brought about with it a variety of challenges to policy-makers and governments, necessitating a paradigm shift in the way policies are formulated.*





It comes as a surprise to many when they hear that IIT Madras has a Department of Humanities and Social Sciences, with many unable to grasp the connection between technology and society. Belying popular belief, technological innovations are rarely the silver bullet solutions to world's problems: a variety of social, political and economic factors influence how implementation of innovations play out in the real world. It is in grappling with this that the role of the departments of humanities and social sciences become critical. In the hands of a social scientist, technology becomes one of the many tools that can make our country and the world a better place and the challenge lies in using these tools effectively.

That's easier said than done, feels Dr. Suresh Babu, Professor at the Department of Humanities and Social Sciences, IIT Madras. One of the biggest problems that India faces today, according to Prof. Babu, is the lack of evidence based policy making by governments. Many government policies do not have empirical evidence to back them up, and this leads to wastage of resources and negative externalities. In an attempt to change this, Prof. Babu has developed a three step procedure for policy making: collecting and generating data, collating evidences and synthesising policies. It is this methodology that Prof. Babu is using to study migration in India, with the end objective being the formulation of policies to ease the problems faced by migrants in our country.



#### ***What exactly is migration?***

Dictionaries usually define migration as movement from one place to another, but that is too broad a definition for practical purposes. Migration can be international or intra-national in nature; it can be due to reasons ranging from lack of employment opportunities to escape from armed conflict; it can be seasonal or permanent or it can mean the movement of entire families or just a few persons, to state a few possibilities.

*“Migration can be international or intra-national in nature; it can be due to reasons ranging from lack of employment opportunities to escape from armed conflict; it can be seasonal or permanent or it can mean the movement of entire families or just a few persons, to state a few possibilities.”*

In India, social and cultural barriers prevented large scale migration of population for centuries. International migration, for instance, faced the taboo of kala pani wherein travelling overseas meant the loss of one's caste, and movement within pre-Independence India was prevented by the linguistic and caste barriers. These factors continued - and still continue - to affect migration, but the rapid economic growth that our country has experienced over the past two decades has, for the first time, unleashed large scale intra-India migration. This brings with it its own set of challenges and has consequences that have not been fully understood, and it is this gap that Prof. Babu is attempting to fill. To put it simply, consequences due to migration can be broadly classified into consequences at the place of departure, at the place of arrival and in the lives of the migrants. These consequences may be positive or negative, and the challenge lies in maximising the benefit of migration in these three broad categories.

#### ***Why do people migrate?***

But to backtrack a bit - if there are a number of problems associated with migration, why allow migration at all? Wouldn't it be easier if the state could just prevent the root causes of migration? According to Prof. Babu, this is not a solution. For one, legally, Article 19 of the Indian Constitution confers upon citizens the fundamental right “to move freely throughout the territory of India” and “to reside and settle in any part of the territory of India” subject to reasonable restrictions. It is hence legally untenable to prevent migration between states: positions taken by political parties like the Shiv Sena and Maharashtra Navnirman Sena fly against the Indian Constitution.



Secondly, earlier models that attempted to explain migration were simplistic: they attempted to explain migration through difference in wages and other push and pull factors. Attempts to control migration using these models have not worked, and as models become more complicated, it becomes increasingly difficult to formulate coherent policies that can prevent migration. For Prof. Babu, the writing on the wall is clear - it is time to accept the phenomena of migration and formulate policies accordingly. This, according to Prof. Babu, requires a paradigm shift in the way we think about migration. Rather than attempting to understand the reason behind migration, there is a need to understand the migrant - their needs, their experiences and their motives.

*“Rather than attempting to understand the reason behind migration, there is a need to understand the migrant - their needs, their experiences and their motives”*

When one considers this from a layman’s perspective, this suggestion does make sense. Let’s take up a scenario where IIT Madras decides to improve the lives of the migrant security guards on campus. Any such endeavor will necessarily require a concerted attempt by the administration and the campus community to understand their experiences, the problems they face and the reason they are working in Chennai, separated from the rest of their families from places as far away as Assam. This shall then help in the formulation of policies that can, for example, help the security guards to not live in cramped, shared rooms and set up mechanisms for transferring remittances to remote areas. However, looking at just the wage differential between Assam and Chennai or deriding the economic opportunities in Assam is not going to lead to this outcome - neither is it going to help understand the reasons behind the migration comprehensively!

One important reason that Prof. Babu put forth for the failure of anti-migration measures was the fact that they are intrinsically tied to anti-poverty measures. To a large extent, it is reasonable to assume that people migrate because of poverty/lack of economic opportunities in their home location and it is hence logical to assume that anti-poverty measures should prevent migration. However, anti-poverty programs in India are intrinsically flawed due to their reliance on the poverty line. A family that avails of Below Poverty Line benefits and just manages to cross the poverty line finds all Government support withdrawn to it. Slipping below the poverty line again is hence extremely probable. To use an analogy from physics - escaping poverty, like escaping earth’s gravity, requires an equivalent of the escape velocity. Migration could very well fit that role.

*“To use an analogy from physics - escaping poverty, like escaping earth’s gravity , requires an equivalent of the escape velocity. Migration could very well fit that role.”*

### ***What should the government do about migration?***

In his quest for evidence-based policy making, Prof. Babu has evolved an extremely stringent research methodology. Nearly 12,000 papers related to migration were reviewed and checked for robustness and quality and this was followed by a meta-analysis that sought to understand the different evidences that were thrown up by different types and forms of data. Quite a bit of Prof. Babu’s research involved fieldwork, and Prof. Babu carried out extensive fieldwork in Sriperumbudur, a satellite town of Chennai that has a thriving Special Economic Zone acting as a magnet for workers from all over India. Chennai Central station was another place that Prof. Babu frequented in order to understand the migrant - the destination and the starting points of migration being important sources of information. In all, Prof. Babu spent nearly 3 years doing field work and another 1.5 years working on secondary literature, and the results are beginning to show.



Let's take a closer look at one such field study. Migrants who arrive at Chennai Central apparently seek out community networks that have been built over time in this city. Belonging to a network is critical for migrants as it is the solidarity amongst community members that ensures that migrants are cared for - very few formal institutional support exists for them. Consider this - if a migrant meets with an accident or falls ill, who is to take care of the migrant and pay for the expenses? In an ideal society, healthcare would be provided for by the state free of cost, but in reality, the migrants are heavily dependent on their community for monetary and social assistance. How exactly then should policies be designed so as to achieve this ideal?

Options for upward social and economic mobility are also few for migrant workers. An interesting phenomena that Prof. Babu observed was the dispersion of migrants that cut across the rural-urban divide. Traditionally, migration has always been associated with cities, but today's migrants can also be found in rural areas. Citing examples of Tamil Nadu and Kerala, Prof. Babu explained how locals of these two states are moving towards higher end jobs, leaving manual labour to migrants from North and East India. What the locals of these states experience is an altogether different type of migration - it is skill-based migration. Educated youth from all over South India descend on Ascendas and other IT parks in Chennai for seeking to make their fortune in the city, and the experiences they have and the problems they face is very different when compared to those of unskilled migrants. How exactly then can low-skilled/unskilled migrants be equipped with some sort of skill-based training to allow them upward social and economic mobility?

A significant number of migrants move around with their families, and this affects the education of their children. Prof. Babu narrated the story of a group of seasonal Bengali migrants in Tamil Nadu whose children refused to attend a primary school run by the government despite the best efforts of the school headmaster. In the end, what actually drew the children in was the hiring of a Bengali speaker as a temporary faculty in the school, but by the time the kids settled in, it was time to move again. How is the state supposed to enforce the fundamental right of children to primary education in such cases?

Prof. Babu acknowledged that there does not exist any silver bullet that can address these varied policy goals. However, this does not mean that there are no measures that can be taken. Prof. Babu emphasized the need for data on migration, and the only way that this can be obtained is if the state starts collecting the same. The cornerstone of evidence-based policy making is the gathering of evidence and this requires the state to expend resources into the creation of a migrant database. Policies that exclusively look out for migrant welfare are also needed - as stated earlier, clubbing the "migrant problem" with other policy measures will not work. Improving benefits of migration also needs an integrated national policy. Migration occurs across states and it is neigh impossible for multiple states to coordinate between themselves and formulate coherent policies. Sustained and long term investment needs to be made in this area to reap dividends, and this too will be aided by a national policy. Access to formal credit would also go a long way in making the lives of migrants better, according to Prof. Babu.

What is needed today is a completely new paradigm to policy formulation. Evidence-based policy making holds the key to tackling the challenges that India faces today, especially a multi-faceted challenge like migration. The most serious impediment to this is the lack of reliable, robust data and it is here that the role of the state becomes critical. The problem of migration also highlights the need for an inter-disciplinary approach to tackling real-world problems: technological innovations and solutions need to be backed by solid research in sociology and economics to be effective.



**Venkataraman Ganesh** (*Author*)

Venkataraman Ganesh is a final year student pursuing Development Studies at the Department of Humanities and Social Sciences. Passionate about development, politics and philosophy, he is trying to make the most out of the last few months he has in insti.



An economist with nearly two decades of experience in development and public economics, **Prof. Suresh Babu** has been part of innumerable Government projects aimed at solving some of the most challenging problems that India faces today. From being a consultant to the World Bank to being the person in charge of monitoring Sarva Siksha Abhiyan (the Central Government's flagship project aimed at Universalization of Elementary Education) in Tamil Nadu, Prof. Babu has had first hand experience in drafting development policies and strategies and his enormous experience is reflected in the way he speaks of development and economics.





# Drumming Out Defects

## *Non-invasive Techniques for Structural Health Monitoring*

by Sharmila Balamurugan

*We have used non-invasive techniques in the medical industry for a long time. For instance, we use ultrasound to monitor the health of our internal organs. In this article, we see how scientists now use ultrasonic waves to non-invasively probe mechanical structures for defects.*



Sensational news about structural disasters seldom inform us of their slow and almost invisible causes. However, several catastrophic incidents share quite a humble and prosaic beginning.

In 1842, one axle snapping in a 16-carriage train led to the loss of at least 50 lives in Versailles, while a single crack in the wheel of a high speed train led to the death of 101 passengers in Eschede in 1998. A crack in one of the six support structures of a Norwegian oil rig led to its capsizing, killing roughly 200 workers in 1980. And one leaky pipe in Bhopal in 1984 caused one of the worst industrial disasters mankind has seen. Flood caused by a molasses tank collapse in Boston in 1919, and De Havilland Comet plane crash in 1954 are some of the catastrophes that stem from a cause which you can hardly perceive and which grows so slowly, but just as steadily.

Catastrophes can start as, or be caused by, something as small as a crack in a huge engineering structure. As the adage goes “all for the want of a horseshoe nail”, industries across the globe lose about 2-3% of their GDP to corrosion in their metal structures. To prevent loss of lives and resources, regular maintenance is mandatory. But maintenance necessitates shutting down of entire processes and factories. This spurs the need to find an optimum frequency of invasive inspection, and to develop noninvasive monitoring techniques to prevent loss of productivity. Moreover, in the case of large engineering structures such as railway lines, nuclear reactors, and cross-country oil pipelines, searching for possible cracks in their metallic structures is like searching for a needle in a haystack. Or rather, like searching for an unknown number of needles in several haystacks, says Prof Krishnan Balasubramaniam, of the Department of Mechanical Engineering at IIT Madras.

The professor tells us that in the year 2009 alone, the southern railways of India recorded finding as many as 2000 fissures in their railway lines. A fissure in a railway line is a complete perpendicular crack along its width. Even if only one in every hundred fissures has the potential to develop into a fracture that can cause damage, there is a significant risk factor that we are posed with. A proposed solution for structural health monitoring is occasional inspection with the help of electronic sensors. This generates a large amount of data, which can be processed using methods like deep learning to give an indication of the health of structures.

Prof Balasubramaniam heads the Center for Nondestructive Evaluation (CNDE) at IIT Madras, which has done pioneering work in this field. Prof Balasubramaniam has worked for more than 25 years in this field, and is at the helm of several startups, that have been incubated by IIT Madras, to work with industries to manage the risk of catastrophic failures. Two of these are Dhvani Research ([www.dhvani-research.com](http://www.dhvani-research.com)) and DeTect Technologies ([www.detecttechnologies.com](http://www.detecttechnologies.com)), that work on building probes for detecting structural defects, especially in hostile environments.

Corrosion is one of the leading factors affecting the health of structures. Prof Balasubramaniam explains that corrosion needs three important ingredients, namely, the metal which gets corroded, water mixed with just enough minerals to catalyse the process, and oxygen. For example, every street light support structure is likely to suffer corrosion at the point where it comes in contact with the ground. The life of this structure can be prolonged by strengthening the base with a layer of concrete, which prevents the metal structure from getting in contact with water.



*Example of corrosion in a pipe*

But things are not so simple when it comes to larger structures and buildings. Corrosion can happen in regions which may not be visible or easily detectable. Hidden corrosion is like a disease that eats away the strength of a structure. Therefore, timely diagnosis helps in



helps in mending the structure, and is done using several kinds of probes. Prof Balasubramaniam's team works on probes that use acoustic signals and thermal imaging. He gives us an apposite analogy: similar to a doctor listening to a patient's heartbeat to detect abnormalities, sensors use acoustic probes to detect abnormalities in reflected sounds, or do thermal imaging which is quite like using a thermometer. Ultrasound and X-ray imaging is just as prevalent and useful in structural health monitoring as in diagnostics.

Prof Balasubramaniam's lab and startups use "guided" ultrasonic waves to detect corrosion. Guided waves (as the name suggests) are waves that propagate in a structure such that they are guided by its boundaries. Fiber optic cables are a well known example, carrying guided light waves. Hence, it is obvious that any structural defects will be reflected in the ultrasonic waves that are guided by the structure. In this manner, devices that monitor the transmitted waves can pick up signs of these defects.

With experience, one is able to gain information about the approximate size and severity of the defect. To automate and standardize such analyses, the teams are building near-real time modelling to gain information about these defects from the transmitted ultrasonic waves. They make use of inverse models which try to reconstruct these defects from the recorded data. Monitoring devices that work with low frequency guided waves are developed by DeTect Technologies to check for large defects over extended areas. The device is permanently installed and is used as a continual health monitoring system, which regularly records data of the entire structure.

Devices with high frequency guided waves are used by Dhvani Research to check for corrosion and small defects. A drawback of finer measurements is that this can monitor only over local regions. This technique is used during inspection. With extensive use of robotics, regions which are quite inaccessible to us are also examined. Prof Balasubramaniam recounts an example of how the technology developed in his lab and used by Dhvani Research checks for structural defects in the base of oil tanks. He tells us that conventional methods for this purpose require emptying the entire tank and long shutdown periods, resulting in heavy expenditure. Their technology, on the other hand, checks the base for cracks from the outside of the structure, without disrupting the functioning of the facility.

Industry-level robustness with extremely low possibilities of false triggers have become the guiding mantra for these startups. DeTect Technologies was chosen by Economic Times as the Best on campus in Startup awards. The technology that the research team at IIT Madras has developed, and which the startups have perfected, is now being used in around 12 countries, mostly in oil and gas industries. Prof Balasubramaniam points out that this success was possible only because the startups put in gruelling effort to get the robustness and perfection required in industry over the idea proposed by the research team. He tells us that in research and in the industry, it is very important to get one's hands dirty and feet wet in the field, literally.



*Non-destructive evaluation of the base of an oil tank*





**Sharmila Balamurugan** (*Author*)

Sharmila is a research scholar who works in the area of quantum dynamics in the Department of Physics. She loves to read and write, especially when there is a stock of sinfully rich snacks kept beside her.



**Prof. Krishnan Balasubramaniam** is a Chair Professor in the Department of Mechanical Engineering. His research interests are ultrasonics and acoustics, structural health monitoring, micro and nano imaging, nondestructive evaluation, materials characterisation, and wave propagation. He also heads the Centre for Non-Destructive Evaluation (CNDE) at IIT Madras.



*Prof Balasubramaniam, his collaborators, and students of CNDE*



# Thermodynamic Charting of Materials Space

by R Mythreyi

*If all materials in the universe lived in one country, thermodynamics will form the government. Every aspect of a material's existence and the changes it undergoes, no matter if it's a pure element, compound or solution, is governed by the laws of thermodynamics. Building from the clear rules that have been laid out by thermodynamics, Professor Hari Kumar from the Department of Metallurgical and Materials Engineering, and his group members, use novel methods to simplify the process of providing useful insights to many engineering materials by generating 'Phase Diagrams' - one of the most indispensable tools in a material scientist's arsenal.*





Elements and compounds have phases like solid, liquid and gas but phases can no longer be clearly distinguished in this manner when it comes to solutions. A simple example will be a solution of sugar in water. When we have pure water, we have one phase - liquid water. Similarly, just sugar is one phase - solid sugar. However, when we dissolve some sugar in water, they mix completely and we once again have one phase - sugar solution. If we keep adding sugar, we reach a limit beyond which sugar can no longer dissolve in water (called the “solubility limit”), and the solution is said to be saturated. Any extra sugar that we add to such a solution will precipitate out as a separate phase - solid sugar, giving us two phases in the mixture - solid sugar and sugar solution. The same phenomenon is observed in alloys (an alloy is a solution of different metals). One element can dissolve another element to form a single “phase”. However, there can be a “solubility limit”, beyond which a second phase of the alloy appears. There can therefore be many different phases even when only two or three elements are involved.

What is a phase diagram? When I ask this question to Guruvidyathri, a doctoral student working in this group, he shows me a “Phase Diagram” for food. He tells me enthusiastically, “A phase diagram is not a two-dimensional graph, where there’s a one to one relation between the X and Y variables. Phase diagrams are more like maps, where there are at least two independent variables that we can change to observe different states of existence. To put it simply, consider a “phase diagram” of food (Figure 1), where we can control “time” and “money”. The kind of food that you can eat, the state of existence, depends on the time and money you have at the moment, your (hopefully) independent variables.” The phase diagrams for material systems are similar. The most commonly used phase diagrams give a map of the stable phase the system exists in, the state of existence at a particular temperature and composition of the system, the independent variables.

### The Need for Phase Diagrams

To understand the need for phase diagrams, let’s imagine this situation. Suppose that you’re to meet your adventurous friend living in an unknown city in a far away country. You reach the city, equipped with some landmarks shared by people who have already been to the place. However, only when you reach there do you realise that everything you know about the place seems scattered, leaving you unsure as to where you must go. As you go from place to place looking for the destination, a kind passer-by gives you a map of the whole city. Relieved, you are now able to quickly find the correct spot and are on your way to meet your friend. Your situation before you knew about the map is not much different from what a metallurgist working on alloy design faces. The applications of an alloy is dictated by its properties. All of us know about the periodic table and the different elements in it. It is not possible to try out all the ways to combine elements to form alloys as the number of combinations is simply too large.

We can now see that metallurgists and material scientists need charts giving them a starting direction to solve many problems. These charts are called phase diagrams. Professor Hari Kumar and his group work on making sure that phase diagrams are available for important engineering materials. For example, by virtue of their high hardness and wear resistance, transition metal nitride coatings are of great interest for cutting and forming tool applications. Titanium, Zirconium and Nitrogen (Ti-Zr-N) is one such important material system. Soumya Sridar, another doctoral student in the group, works on the thermodynamic modelling of these transition metal nitride systems in order to get the phase diagrams. She says, “Knowing the phase equilibria information is crucial for understanding phase evolution in the material and for fine-tuning the chemistry of these coatings to enhance their properties”.

### A Simplified Analogy for Phase Diagrams

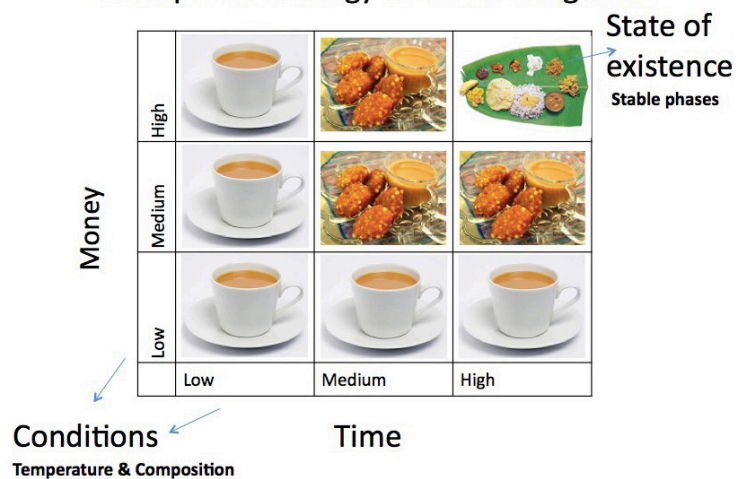


Fig. 1: A ‘Phase Diagram’ analogy for food.  
Money and Time are the independent variables.  
The kind of food one can eat is the ‘stable state of existence’





### **Computational Thermodynamics**

This idea of thermodynamic ‘modelling’ is novel. Phase diagrams were generated only based on experiments in the earlier days. Since there are at least two independent variables, to get each phase diagram, researchers would perform systematic studies on varying amounts of materials in a particular system and would obtain the stable phases that exists at a given temperature, pressure and composition of the alloy. Looking at the complex phase-temperature-composition space that materials span, it was realized in early 1950’s that it’s quite a challenge to probe all of it through experiments alone. It was known that using thermodynamics to generate phase diagrams would be more efficient and powerful. With the development of computational tools in the 1980’s, the field of “Computational Thermodynamics” emerged and rose in popularity. These clever combinatorial techniques remove the sole dependence on thousands of painstaking experiments. This method of CALculation of PHase Diagrams is called CALPHAD. However, being a combinatorial technique, CALPHAD requires inputs that come from either very careful experiments in selected regimes of composition space or other computational methods. Therefore, in CALPHAD, experiments and computation complement each other.

Thermodynamics is the study of transfer and conversions of energy that happens in different processes, including mechanical, thermal and chemical reactions, and the resulting changes. Based on the conditions in which a process occurs, there are different measures of energy that can be analyzed. One such measure is called the Gibbs energy, denoted by the symbol ‘G’. In thermodynamics of engines, it’s often called the useful energy that can be extracted from a system at constant temperature and pressure. The entity that restricts the complete extraction of energy is called entropy, denoted by ‘S’. Entropy is a measure of randomness. We can quantify the energy that gets dispersed out randomly, thereby becoming unavailable for useful extraction, using entropy. If true magicians existed, the energy that they will have to provide through their magic to pull a rabbit out from a hat is the Gibbs energy of the rabbit. Thus, ‘G’ (Gibbs energy) will be ‘U’ (Internal energy, for the atoms in the rabbit’s body),



*Fig. 2: Understanding Gibbs Energy intuitively to see why it must get minimised at equilibrium*

added with ‘PV’ (Pressure times Volume, energy to move the atmosphere away and create space for the rabbit) and subtracted by ‘TS’ (Temperature times Entropy). This is illustrated in Figure 2. Thus, Gibbs energy is a function of the state of the system and the state is determined by variables like temperature, pressure and composition. Being a fundamental law of thermodynamics, in our universe, all processes lead to an increase in entropy. When all systems tend to increase the entropy, it also means that all systems try to minimise their Gibbs energy, obtaining a stable state or ‘equilibrium’. It is one of the crucial ideas behind generating phase diagrams through CALPHAD because this gives information about which phases will be present at equilibrium at given conditions.

### **Using CALPHAD to get Phase Diagrams**

To get a phase diagram using CALPHAD, we need to first find out all possible phases a chosen system can exist in. This depends not only on the number of components in the system, but also on the type of components and their mutual interactions. Once we know which phases can potentially form, the next step is to get the Gibbs energy function of each of the possible phases. This step is called the ‘Gibbs energy optimisation’ step. Here is where CALPHAD takes in inputs from other methods.

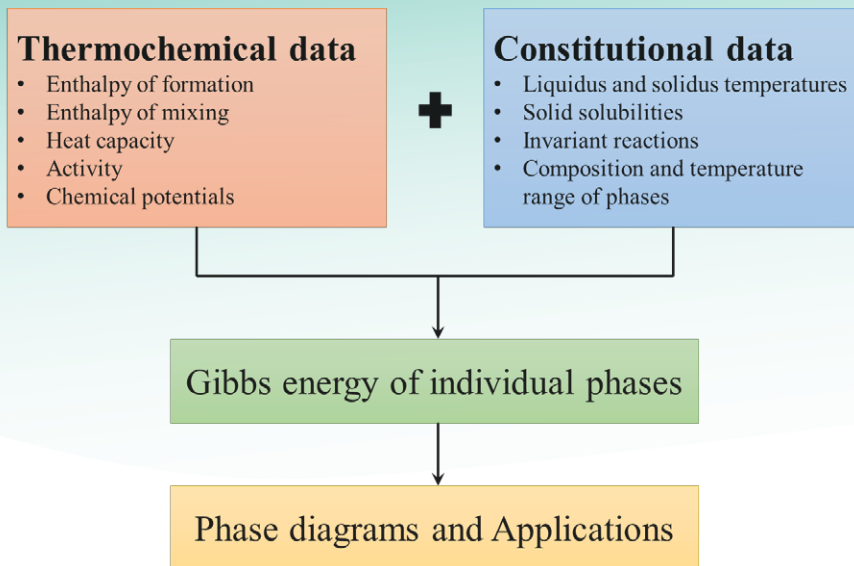


Fig. 3: Flow of information in the CALPHAD method

to the what we observe when we rub a plastic ruler with fur and use it to ‘attract’ bits of paper. The difference is that, in DFT, the interactions are based on quantum mechanics and are more complex. Once we get sufficient inputs, CALPHAD can give us a Gibbs energy function for all of the phases present through a careful optimisation exercise with some constraints included. After this, thermodynamics allows us to calculate the ‘equilibrium’ by minimising the optimised Gibbs energy expression. This minimisation can be thought to be a competition among the different phases to reach the lowest Gibbs energy. We can expect more than one winner out of this competition because thermodynamics allows multiple phases to reach a stable state that has a Gibbs energy lower than what the individual phases can reach on their own. At the end of this minimisation, we have information about the best combination of phases at a given state. This information is sufficient to construct the phase diagrams. As with any computational technique, some experiments are needed to corroborate the results obtained. Figure 4 is the phase diagram of Zr-N, is an example of such a comparison.

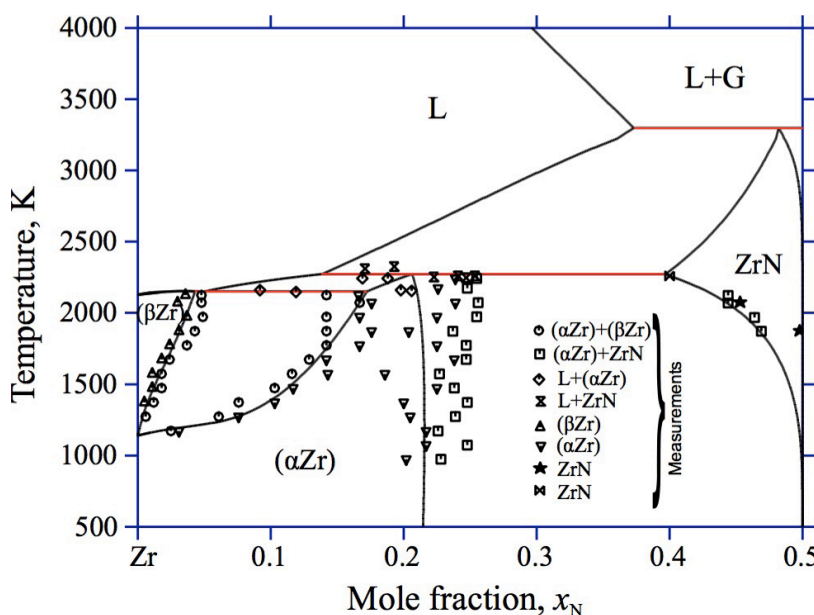


Fig. 4: Comparison of calculated Zr-N phase diagram and experimental data. Such a comparison validates calculations.

### The Advantage of Computational Thermodynamics

The real power of computational techniques can be realised only when we look at alloys with many components and the serious scaling up that happens to the numbers involved. When we consider that there are around seventy useful engineering materials, nearly all the binary (two elements) combinations have been studied and around two thousand binary phase diagrams are accessible in form of handbooks or databases. This is a result of generation of phase diagrams through both experimental and computational methods. If we add one more element to form ternary (three element) systems, the number

of phase diagrams possible explodes to around fifty thousand. While some of ternary phase diagrams have also been generated so far, the number is much lower than fifty thousand. A new emerging trend in alloy design is the study of High Entropy Alloys, also called HEAs. In HEAs, four or more different elements are combined in equal



proportions to form new alloys. With the inclusion of these many elements, we can see that the numbers are just too big. If one starts a purely experimental program to generate all such phase diagrams, it's going to be a very time consuming and difficult task. Here's where CALPHAD comes in handy.

The highlight of the CALPHAD method is that it doesn't require experimental data generation for four or five component systems; it works by extrapolation. The generated Gibbs energy functions of the lower order systems can be extrapolated to higher orders (four or more elements) based on some geometric methods. This extrapolation is very reliable because of two main reasons - one physical and one mathematical. When we look at the number of phases in unary (one element) systems and number of phases that are new in binary systems, the difference is big. A binary system can sometimes even have fifteen to twenty phases possible. But while creation of new phases is rampant in binary systems, the number of new phases decreases substantially thereafter. Rarely do find new phases that form in the higher order systems beyond the phases found in the ternary system. Hence, we do not have to extend the experimental search beyond three or a maximum of four components. This is the physical reason why extrapolation works in CALPHAD. The other reason is mathematical. The energy functions that are generated through CALPHAD usually have the energy contributions of each phase weighted by the composition of the phase. Composition is a fraction, therefore the unary contributions are multiplied by one fraction, binaries are multiplied by two, ternaries by three, and so on. When a number is multiplied over and over by a fraction, its contribution to the total energy becomes very small. We can safely ignore these terms and this adds to why CALPHAD works well.

### ***Linking CALPHAD with other Computational Materials Engineering Techniques***

Thermodynamics doesn't deal with time, it can only tell us whether a change is possible or not but can't tell us how long it will take to happen. For instance, thermodynamics says that diamonds are less stable than graphite (the same substance that makes our pencil leads) and so diamonds must transform into graphite to reach their equilibrium. But thankfully, the rate of this reaction is so slow at ambient conditions that we don't observe this in the jewellery that we buy after paying lots of money. The rates of reactions are dealt with in kinetics. Most of the time, the engineering applications of a material will not require the equilibrium phase of the material. There may be other useful phases with desirable properties that have useful applications. Since the material is not at equilibrium already, it always has a tendency to transform. But when we use it in applications, it becomes important to look at how long the material can remain in the non-equilibrium state as the changes in its properties due to its transformation could be catastrophic to the application. We will have to know in advance when the material will be exhausted and for this, we perform kinetic simulations. To perform these kinetic simulations, we need thermodynamic inputs. The Gibbs function that we obtained by generating phase diagrams can become inputs to such simulations because though the phase equilibrium information that we got is the primary output of CALPHAD, we can also, in principle, obtain any other thermodynamic property that's related to the Gibbs energy.

The most important difference between other computational techniques used in Material Science and CALPHAD is that it is very simple and one doesn't require very powerful computing resources. This is because it relies on classical thermodynamics and minimisation. In techniques that use quantum mechanics like the Density Functional Theory discussed previously, the time required for calculations in higher order systems scales up very quickly. CALPHAD can handle such complexities fairly well and even multi-component systems up to twenty elements can be worked on using a simple laptop. This advantageous position occupied by CALPHAD in modelling of materials becomes instrumental in stringing different order systems together. One can model the lower-order systems using other techniques, and take those inputs to develop the necessary Gibbs functions for higher order systems using CALPHAD and proceed to calculations of such systems. Because of the opportunities to do more than one type of computation, CALPHAD, apart from being useful, is an interesting domain to pursue too.



**What lies ahead**

CALPHAD has grown into big community worldwide and every year a conference (called “CALPHAD”), brings people who work in the field together. During the early years of Computational Thermodynamics, there were new codes that were written to perform the required calculations. Some of the codes that started out as open-source, soon became commercial and now there are softwares like Thermo-Calc and Pandat, and Open Calphad is an open source distribution. The software provide holistic environments to use the CALPHAD approach. Their usage is growing in the industry as well and most people have now realised that computation along with careful experimentation can bring down the time to develop new materials for applications. There are no other groups in India that’s working extensively on Computational Thermodynamics. This makes Professor Hari Kumar’s group unique.

One of the key contributors to thermodynamics, Lord William Thomson, known better by the name Lord Kelvin, said in 1900, “There is nothing new to be discovered in physics now. All that remains is more and more precise measurement.” Nearly all the physics we now know to be right was discovered after 1900. Thermodynamics is an exception and it has stood the test of time. But from what we’ve seen so far about the work in Professor Hari Kumar’s group, thermodynamics has become more powerful by adapting to improving technology. Thermodynamics, the old dog, has learnt new tricks.

**R Mythreyi (Author)**

Mythreyi is a third-year undergraduate student in the Department of Metallurgical and Materials Engineering. Being the kind of person who spends more time researching productivity than being productive, her compelling love for books and music has recently taken her on an exploration of cognitive psychology, rationality, the brain and classical music. She finds it thrilling to try and unearth correlations between many different things that capture her enthusiasm. Oftentimes, she finds energy through writing twisted and complicated sentences. She hopes to pursue research in Computational Materials Engineering.



**Dr. K. C. Hari Kumar** is a Professor in the Department of Metallurgical and Materials Engineering at IIT Madras. He is an Associate Editor of Calphad (an Elsevier journal) and a Key Reader of Metallurgical & Materials Transactions A (a Springer Journal). His research interests are Gibbs Energy Modelling of Materials, Applications of Density Functional Theory in Materials Science, Modelling of Diffusion Controlled Phase Transformations and Applications of Thermodynamics in Process Metallurgy.



*Prof. Hari Kumar and his Research Group*



# *What the voids have in store*

*by* H.V. Ragavendra

*What makes the star-studded night sky serve as a cue for pure curiosity and trigger a subsequent train of philosophical thoughts? Well, the appeal of a starry night are the stars of course, you may say. But do you know that the voids that seem like a humble background are as interesting as the stars themselves? While the stellar objects usually steal the show in public discussions of science, Dr. Aravind, researcher of the composition and dynamics of molecules of the Interstellar Medium (ISM), raises the curtain on the play of atoms and molecules that are largely in the dark, well, literally.*





Dr. Aravind and his research scholars, who form the group of Atomic and Molecular Physics in Physics Department at IITM, have been actively studying in their lab, the nature and behaviour of molecules that are found in the vacant spaces between stars. The Interstellar Medium usually contains highly energetic protons, electrons, electromagnetic waves and multiatomic anions. These negatively charged anions made of several elements are the ones that give us information about the voids, like how sparse they are and what chemical reactions one can expect to occur amongst them.



Dr.G.Aravind and his students:  
Saroj Kumar Barik and Roby Chacko

The usual method to test the presence of a molecule or an ion in ISM is to measure the wavelength of the light emitted by it in the lab and compare it against the wavelength recorded from astronomical observations. If the molecule emits light same as the observed ones, one can go ahead and study how it reacts in such an environment. This method is called 'laboratory astrophysics', where you simulate astrophysical environment; put in the molecules that are likely to be present in actual astrophysical environments and see what the reactions and end products are in the simulated one. The professor and his team address two crucial aspects of this study. The first is to identify the structure and energy levels of the constituents of ISM and the other is to study their dynamics by identifying the reactions between them. They employ a variety of techniques to perform these two studies.

The first hurdle in the studies of anions is their synthesis. Neutral molecules are happy the way they are and allergic to negativity, that is, they do not easily accept another electron and become anions. Even when ionized, the anions easily break apart when excited. One way to make neutral ones pick up electrons is to let them expand faster than the speed of sound in a vacuum chamber, which is evacuated to a pressure of around 1 part in 100 million of normal atmospheric pressure, and hence get cooled. This is called 'supersonic cooling'. This cool gas is subjected to high voltage electrical bursts. This makes the molecules pick up electrons and turn into negative ions. The idea of cooling before ionizing makes sure the ions do not get agitated and break apart. But there is variety in the anions produced; so we must select the ones we want from this collection.

This business of selecting the desired type of anions is taken care of by a crafty device called 'Time-of-Flight-mass spectrometer'. This works on the principle that for a given force, heavier ions move

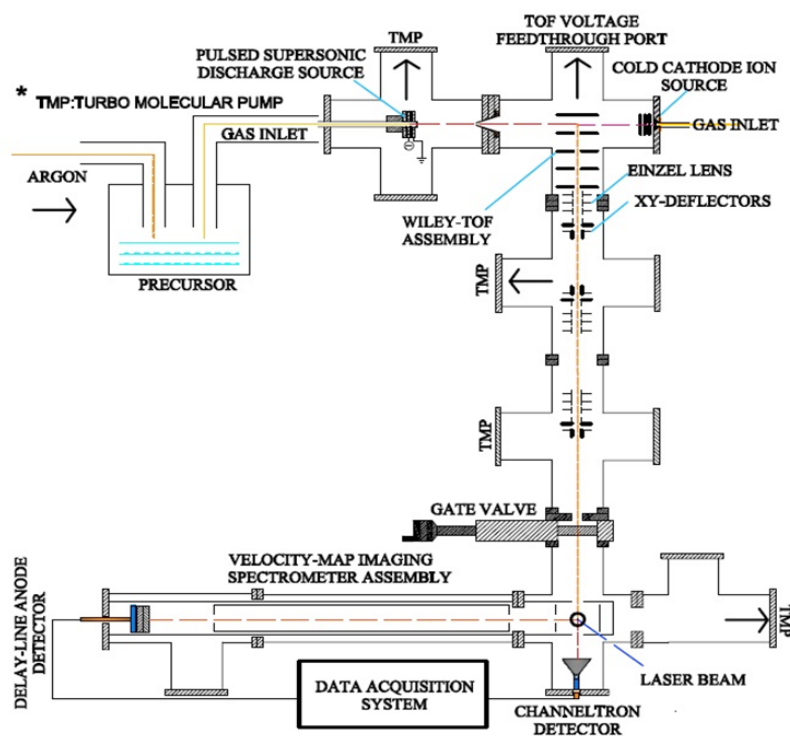


Fig.1: Schematic of PES setup complete with Mass-time spectrometer and VMI. The PES, which forms the top part of the figure, works like this: The ion source, the repelling electrode and mass-gate are supplied with electric potential in the form of a train of pulses. The ion source containing supersonic cooler and an array of cathodes produce anions in bunches corresponding to voltage pulses. The repeller whose pulses are delayed with respect to the source pushes the anions through the time of flight chamber. The mass-gate whose pulses are further delayed traps the required anions. The delay of the mass-gate with respect to the repeller is the one that selects the desired mass from the variety produced. All these delays are within one pulse range, such that the entire sequence is repeated for each pulse and a steady supply of anions is achieved.





This means that if you know the mass of a particular anion you know the time it takes to fly across a given length. So, different masses arrive at different times at a particular point in the detector. To be exact, the time of flight of anions with 1 unit negative charge, is proportional to the square root of their masses. That means, if it were twice massive, it will be 4 times slower; thrice massive, 9 times slower. Hence the spectrometer is tuned to let the unwanted masses to fly off and when the ion of required mass comes, a mass-gate made of meshes with electric voltage is turned on to trap it. All this happens in nanosecond scale (a nanosecond is one part in a billion divisions of a second) as the device can be precise enough to identify anions arriving by delays as small as eight nanoseconds.

With the required anions produced and filtered thus, the research group proceeds to study the energy levels of the anions. For this, photons of suitable energy are made to hit anions and kick out the extra electron from it. Quantum mechanics dictates that the anion's energy is quantized, that is, it can only have certain energy values, not arbitrary ones. So, knowing the photon energy and by measuring the electron's kinetic energy, we should be able to say what the energy levels of the anions are. Most of the anions have utmost one electronic state that is stable against electron detachment. The excited states of anions eventually detach an electron or dissociate into neutral and negative fragments. Such excited states, called 'resonances', play a vital role in Astrochemistry, as they influence the way a molecule fragments. These resonances provide insights to the population of molecular species in the ISM, as we shall see, in one of their recent study. Note that we start with neutral molecules first, ionize them, then kick the electron out and study it to understand the anion. In a sense, the electron acts as the messenger that is deployed to collect information about the anion it was made part of. This technique of inferring energy levels of anions using electrons kicked out by photons is called Photoelectron Spectroscopy (PES). So much to get a single number, the energy of the electron? Well, there is more. It would be better if we get the velocities (both speed and direction) of the electrons emitted from a group of our anions, not just their kinetic energy. This idea of velocity mapping is the state-of-art technique for studying anions.

The professor reminisces building a Velocity Map Imaging device (VMI) for anions, during his days of Ph.D., which happened to be the first of its kind in India. "The process of velocity mapping, even for anions, is extremely tricky. But doing the same for electrons brings in its own host of problems", he says, regarding his pursuit of this particular study ever since. To device a VMI setup for electrons, one has to exclude all possible external fields, even the feeble ones like Earth's own magnetic field and those from materials like screws and bolts in their vicinity. This is because these are enough to deflect particles as light as electrons from the expected trajectory. So the chamber covering the path of electrons has to be shielded with -metal (an alloy of Nickel and Iron), which can shield almost all the stray magnetic field. There are several such precautionary measures to be taken and sensitive fine-tuning to be done to achieve VMI of electrons. Such a delicate yet indigenous construction that is currently hosted in this lab, has been a real achievement for the group. This full setup of PES, i.e., VMI combined with Mass Spectrometer, as shown in Figure 1 is for electrons emitted by anions when impinged with laser light. To put the working of the device in simple terms, it has electric field lines configured in a specific shape in space such that when electrons pass through them, they get pushed according to their speed and direction of motion. In a sense, the field categorizes the electrons going through them as per their velocities before they hit the screen. This results in electrons of a given

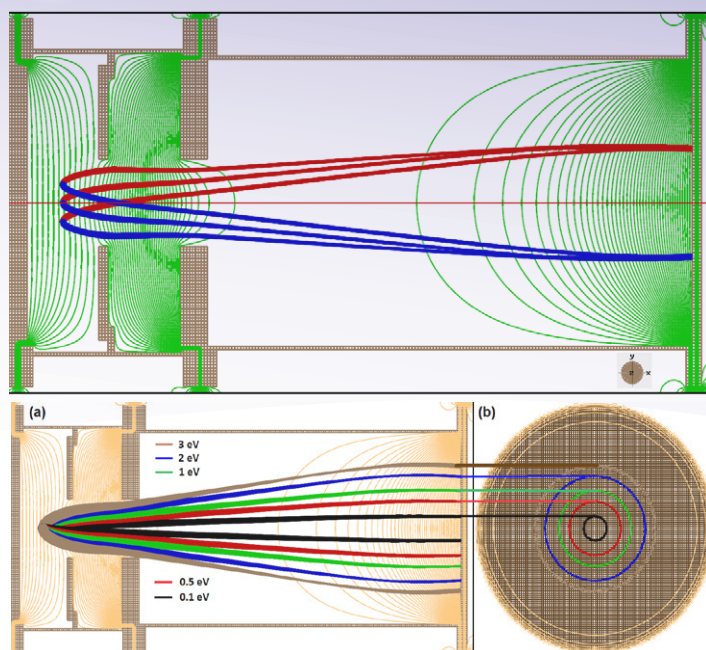


Fig. 2: (Top) Electric field configuration in Velocity Map Imaging setup  
Fig. 3: (Bottom left) Electrons of given energy having a unique trajectory  
(Bottom right) Detector screen with rings corresponding to trajectories

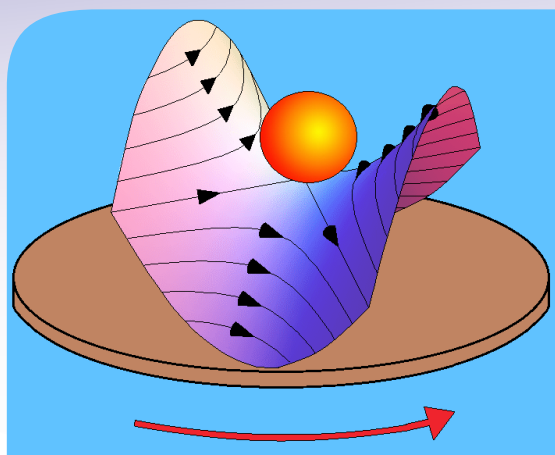


Figure 4: Effective potential of a 4-pole ion trap

speed and velocity direction falling at a particular point on the detector screen. This configuration is illustrated in Figure 2, where the green lines are field lines and the blue and red lines are the paths of electrons with the same speed but opposite orientation. This means that if you know the point in the screen where the electron has hit, you know its speed and the angle it made when it hit the laser. This at the end of the run, presents a visualization of the vector field of the velocities of electrons in the screen. Of course, since the screen is two dimensional, we get the 2D picture or a projection of the vector field. A typical detector screen at the end of the run will look like Figure 3. Here, the electrons recorded in a given ring correspond to the same speed and hence the same energy. The radius of a ring is proportional to the speed of electrons forming it; larger the ring, higher the speed. A point on the ring gives the angle the velocity vector makes with the laser axis. This visual depiction of the velocity field of the electrons, on further analysis, gives the complete information about the state of the anion. The interesting aspect is that because of the time scale and precision of the instrument described, the production of ions and the velocity imaging of electrons is done in a single run of the experiment.

Understanding the composition and energy levels of anions is just one part of the group's aim. The second phase is to discern the dynamics of these anions: how they react chemically amongst themselves and what products they give out. For this purpose, the team has indigenously built 'ion trap'. Ion traps, in general, are considered a boon for spectroscopic analysis because they do what is usually considered very difficult and therefore circumvented in most studies - they hold the anions in a reasonably small volume. With no demand for any increase in timing precision or indirect studies, one can put the anions inside an ion trap, cool them and see them react with the environment you design.

But it is almost impossible to keep a charge at rest using an electric field. They are easily attracted or repelled out of their position by other charges or forces in their vicinity. Well, then how does this trap "trap" ions? The schematic, given in Figure 4, shows how it works. The rods are supplied with an electric potential that varies with time periodically, in such a fashion that alternative rods have a constant offset in their potential at any time, which effectively places the ion in a rotating saddle as shown. In simple terms, when the negative charge sees positive potential in a rod and moves towards it, the potential is switched to the next rod. This makes the charge to change its direction and by the time the change occurs, it is again switched to the subsequent rod. By timing this sequence precisely, the charge is effectively trapped in a region around the center of the cylindrical chamber. This tantalizing application of electric potential - the pushing and pulling of the poor ion towards a different rod at subsequent instances so that the net displacement of it is zero, gives us the time required to conduct experiments on it.

The ion trap, as depicted here in Figure 5, has twenty-two rods and again one of its kind in the country. It produces an effective potential as shown in Figure 6. This trap, loaded with the candidate species (usually a Polyaromatic Hydrocarbon), is to be cooled to around 4 Kelvin, using liquid Helium, which is the typical range of temperatures of ISM. Then, it can be made to react with other species of candidate gases and the products formed are checked at different time scales. The products when identified with a mass spectrometer will tell us about the probability of their occurrence in ISM. They

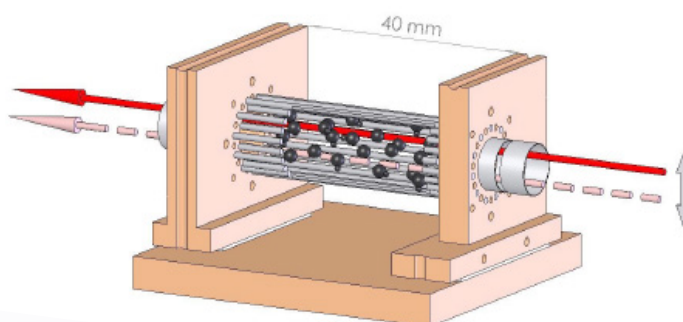


Figure 5: Illustration of an Ion-trap





also tell us the typical time taken for a reaction to occur at these extraordinary environments compared to the usual rate of reaction in lab conditions. This setup is being equipped with sensors and after calibration, it will be employed to study Fullerene cation ( $C_{60}^+$ ), a species of molecules which is found to be abundant in ISM recently.

Such studies of reactions between different candidate species are exciting and as they sometimes suggest the presence of unexpected species of molecules or ions in space. They also help solve the mysterious presence of some rare anions in interstellar voids, whose formation mechanisms are subjects of interesting debates. In addition, they may provide an alternative explanation to the existence of species that were hitherto known to be of different origin. One such instance is the explanation for the abundance of  $CN^-$  in ISM. So far, they were known to be formed in the extremely hot shock waves following supernovae explosions that mark the end of giant stars. But, Dr. Aravind and his Ph.D. student Roby Chacko, say that they have witnessed an exciting result concerning formation of  $CN^-$  through an alternative and relatively cooler mechanism - through the dissociation of one of the heavy molecules in its ionized and unstable, excited state (recall the resonance states described earlier), at temperatures much lower than that of supernovae. Such new physics is what typically motivates further pursuit of this work. One can never know what exactly happens in such strange environments that we are probing.

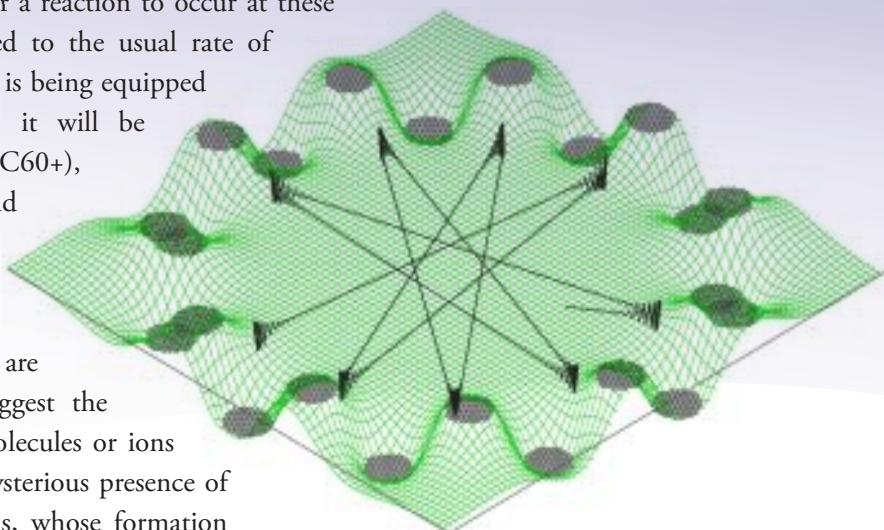


Figure 6: Effective potential of a 22-pole ion trap. The black lines mark the possible trajectory of an ion.

The future outlook for this project will be the assembling of a full-fledged apparatus of anion analysis in a series of Ion Source - Mass spectrometer - Ion trap - Mass spectrometer. A setup of this design will at once produce anions, mass-select the required species with the first mass spectrometer, trap the selected anions and make them react with a supplied environment and identify the products coming out with the second mass spectrometer. A

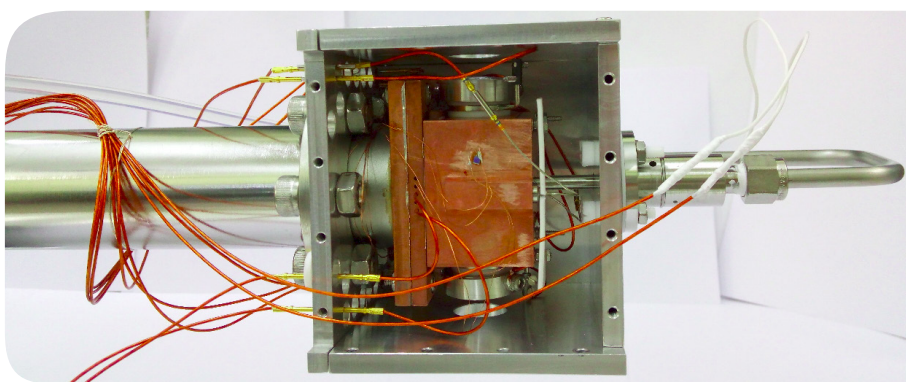


Fig. 7: Picture of the Ion-trap in the lab, attached with different sensors

desirable extension to this setup will be ion benders placed on either end. This will enable placing a laser source along the assembled line of spectrometer-trap-spectrometer that will open the doors to study ion-photon interaction along with ion-neutral and ion-ion interaction. This addition may not take long, as the ion bender has already been devised by one

of the project students of the lab. Such an environment of simultaneous development of apparatuses and sequential conducting of experiments through different projects, yet with a common objective and a clear coordination among them, makes sure the members of the lab know their part in the larger picture to contribute efficiently.

“That is the thing about the students”, says Dr. Aravind indulgently, “They have the potential to do good quality research; it is just a matter of showing them the right direction”. This is evidenced by the number of devices populating the lab in different stages of their building and assembly. These stand as souvenirs of the patience and perseverance demanded by such works of ambitious nature. “For instance, the calibration of the instruments like mass spectrometer



alone can take up to two months”, says Roby Chacko, signifying the time involved to assemble, test and run the devices developed by them. Accuracy and consistency of the results are of paramount importance. However, from what Roby says, there is always a thrill in this research of discovering a new phenomenon or materializing something that was completely speculative. And this is what, we gather, drives Dr. Aravind’s group in their quest to decrypt the darkness of the night sky.



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H.V. Ragavendra is a research scholar working on Cosmology in the Department of Physics, IITM. When his to-do list looks sparse, he tries to expand yet catch up with his to-read list that may contain anything from scientific review articles to a Poetic thriller or a dystopian novel.



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*The research group with their Ion-trap-Mass-spectrometer setup*

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2. *NGS transcriptome data analysis at a glance: finding out the real cause of neurodegenerative disorders*. Source: Diagram by author, created using Adobe Illustrator (AI). Line drawing of brain, from pixabay.com, modified using AI. Neuron-glia communication image from Wikimedia Commons (OpenStax CNX Biology textbook).

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2. Figures 2-7: Prof.Ligy Philip and lab

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1. Image of Ion trap: Photodetachment of Cold OH- in a Multipole Ion Trap” by S.Trippel, et.al., (doi 10.1103/PhysRevLett.97.193003)
2. Images of Rotating Saddle : Dr. Jessie Petricka’s webpage ( <http://physics.gac.edu/~petricka/research/General%20Concept.htm> )
3. and Dr. Holger Kreckel’s webpage ( [http://www.hkreckel.de/ion\\_trap.html](http://www.hkreckel.de/ion_trap.html) )
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