



P-ISSN: 2349-8528

E-ISSN: 2321-4902

IJCS 2018; 6(6): 2751-2756

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Received: 09-09-2018

Accepted: 13-10-2018

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## A journey towards systems biology: Biocomputing of hi-throughput omics data: A national training workshop report-2018

**Gohar Taj, Apoorv Tiwari, Rutash Kumar, BR Singh, Ashutosh Dubey, SD Samantaray and Anil Kumar Gaur**

**Abstract**

Recent years, rapid developments in several omics platforms and next generation sequencing technology have generated a huge amount of biological data about plants. Systems biology aims to develop and use well-organized and efficient algorithms, data structure, visualization, and communication tools for the integration of biological data with the goal of computational modeling and simulation. Plant systems biology studied by some major steps including analysis of gene, protein sequences, and informational pathway, integration of data, and formulating mathematical models that describe the structure of system and its response to individual perturbations. With advances in proteomics and regularly updated open access databases, bioinformatics will contribute to those processes by providing purposeful information of target candidates and correlating this information to biological pathways. More studies are currently being directed towards unraveling the delicate network of interactions that govern cellular and development processes in organisms. Success in this exciting endeavor will be possible only with collaborative and cross-disciplinary efforts in close association with scientists in disciplines such as computer science, statistics, and information visualization. Once this collaboration is matured, it will be possible to understand and predict whole-plant performance in a given set of conditions. Finally, it will be possible to use such models in a predictive mode which can be applied for improving the desirable traits associated with agricultural crops.

**Keywords:** omics, systems biology, plant physiology, GBS, agriculture

**Introduction**

Bioinformatics is a science of 21<sup>st</sup> century and its technological embedding makes this field critically applicable for different fields of sciences including biological, chemical and physical sciences related to agricultural benefit. From technologically-driven wet-lab experiments of biological research, big-data coming out are accumulating at a phenomenal rate. Now the scientists are taking about integrative approaches to come up with big-data of plant, microbes, animal genetics, proteomics and metabolomics (Katam K, 2015) [7]. The ease with that computers will handle an oversized quantity of numerous knowledge at a time and probe advanced dynamics determined, makes computers indispensable to help in scientific research (Garg *et al.*, 2016, Likić, *et al.*, 2010, Taj G., 2011 & 2015 and Yadav *et al.*, 2016) [4, 12, 19, 20, 23].

In the era of fast growing biological data coming out from the – *OMICS* research (genomics, proteomics and metabolomics) from the phenotypic as well as genotypic analysis of many crop plants, live-stocks, microbes, habitats and other interrelated entities, bioinformatics has come forward across the globe to solve the problems of analysis, prediction, management, storage and retrieval of the data to find out fruitful outcome (Sharma *et al.*, 2018, Mochida *et al.*, 2011) [17, 8, 11].

Today, there is a growing need of *OMICS* based approaches for decoding the complexity of biological systems. Omics based approaches having immense potential to study biological systems for novel insights. These approaches have revolutionized the means within which researchers analyze the presence and relative abundance of proteins and expedite the screening and validation method for discovery of drugs/agrochemical for agricultural applications (Likic, 2010; and Rezaei 2012) [12, 15]. Reliable and affordable supply of food is of crucial importance to the progress and stability of human societies. Advent of newer approaches of “omics” sciences and technologies will enable to address several issues and

challenges faced by modern agriculture and also ensure food and nutritional security. Bioinformatics & Systems Biology could be a valuable approach for a systems level understanding of different crop plants (Kumar *et al.*, 2015a & b, 2016; Jill *et al.*, 2009 and Nanda *et al.*, 2011) [9, 6, 14].

Technologies that measure characteristics of large families of cellular molecules (e.g., genes, proteins, metabolites), have been collectively described by using the suffix '-omics' at the end of the name of the characteristic measured. Etymology of the suffix comes from the Latin suffix '-ome', derived from mass or many (Yadav N. *et al.*, 2016) [23]. Thanks to the omics approach of high-throughput measurements are commonly applied specifically genomics, transcriptomics, proteomics, metabolomics and bioinformatics. Further, over 200 '-omics' sub-disciplines have nowadays emerged, including but not limited to epigenomics, glycomics, interactomics, lipidomics, nutrigenomics and foodomics (Yadav 2007 and Rupesh 2012).

In many plant species, the event of omics resources has progressed to deal with specific biological properties of individual species. From these perspectives, the national training workshop has been organized to provide the emerging aspects of plant systems research based on omics and bioinformatics analyses together with their associated resources and technological advances (Rutash Kumar *et al.*, 2018, Avashthi *et al.*, 2014, Mochida *et al.*, 2011) [16, 1, 8, 11].

The emerging advanced high throughput technologies facilitate the systematic study of the complex traits and the regulation underlying the phenotype of the biological organisms. In contrast to the classical research before the post-genomic era, the current agricultural, veterinary and biomedical research tends to investigate the behavior of all system components simultaneously (Bartocci *et al.*, 2016 and Tiwari *et al.*, 2016) [2]. This strategy intends to reveal how the system components collaborate to regulate the system behavior rather than an attempt to identify the individual function of a component. In context of the agricultural research, the systems based approaches have been exploited to explore the biological regulation controlling agricultural productivity (Gaur, M., *et al.*, 2018, Xue *et al.*, 2008, Mochida *et al.*, 2011, Singh *et al.*, 2011) [5, 22, 8, 11].

## Objectives

The major objectives of the workshop were centered around to understand different omics approaches in order to cope up with the simultaneously challenges in agriculture and life sciences areas. In this 4 days national workshop the major objectives that were covered are:

- Analysis of large amounts of omics (Genomics, Proteomics, Transcriptomics, and Metabolomics) data of plant biology through big data analysis computational tools.
- Introduces fundamental and applied bioinformatics research in the field of life sciences.
- Highlights relevant databases, softwares, tools and web resources developed till date to make ease of access for researchers working to decipher plant responses towards stresses.
- Molecular modeling and docking studies for Characterisation of the binding behaviour which plays an important role in rational design of drugs as well as to elucidate fundamental biochemical processes.

## Content and Outline of the workshop

The idea of organizing this training was conceived while we

are feeling lacunae in our knowledge systems biology for agriculture. This put forth a greater Challenge in developing techniques and methodologies through a paradigm shift from the conventional way of research. This approach has higher potential in agricultural, veterinary and biomedical research for identification of important bioactive molecules for various applications. Keeping in view of above, National Training Workshop on "A Journey towards Systems Biology: Biocomputing of Hi-throughput Omics Data" was organized for the benefits of academic fraternity. The organizing team consists of Dr. Gohar Taj (Organizer), Dr. S.D. Samantary (Co-Organizer), Dr. B.R. Singh, Dr. Ashutosh Dubey and staff of Sub-DIC Bioinformatics (Mr. Apoorv Tiwari (SRF), Mr. Rutash Kumar (JRF), Mr. Ganga Datt Sharma, Mr. Ram Pratap Singh and Mrs Neelam).

## The details of contents covered in the workshop were as follows

### Molecular and Structure biology

Studying the architecture, shape, and dynamics of biological micro/macromolecules is paramount for understanding the basic mechanisms that drive the essential processes of all life. Macromolecules such as proteins and nucleic acids carry out most of the functions of a cell, and are able to perform these functions by adopting assemblies of structures under native state conditions. Structural biology is concerned with the driving forces and interactions that determine the three-dimensional shapes and dynamics of bio-molecules.

### Big data analysis

All organisms operate through activating and repressing genes in a coordinated and timely manner between biological conditions. Gene or protein cannot work in isolation. Understanding how interactions are formed and activated at specific time points or conditions is a central part of understanding how specific cells work. With the increase of high-throughput methods it is possible to obtain large amount of data to study a cellular system from complementary aspects more easily. The vast quantity of data produced also enables data re-use and provokes new methods for integration of heterogeneous data.

### NGS Analysis

Intervention and application of NGS data analysis and sequencing technologies in the plant biology by study of different file formats and databases for pre-processing of raw reads and quality control and important role of Transcriptome/Genome/GBS data in Plant systems biology for betterment of agriculture sector

First day of workshop, Registrar of our university Dr. A.P. Sharma inaugurates the workshop with a very informative lecture and said that of Pantnagar University maintain top position in the frontier area of agriculture research and extension since establishment. Green revolution has been successfully initiated by its tireless efforts. He said that the university is doing well not only in the area of agriculture but also advanced area of Life Sciences including Biotechnology, Bioinformatics, Microbiology and Nano-Technology. He describe that future increase in agriculture production in wake of growing demand has to come through mainly productivity enhancements with nutritional security and for that first of all identify hub network of all the genes responsible for important traits and use that network level information for agriculture and animal productivity. These efforts provide help in the development of newer disease resistant, high

yielding varieties and application of emerging technologies such as hybrid technology, genetic modification, and computational approaches are certainly the viable options to raise production.



**Fig 1:** Inaugural Function of the four days national training workshop

Prof. A.U. Khan, a renowned scientist from Aligarh Muslim University, recognized as eminent researcher in the field of antimicrobial resistance was the Guest of Honor. Dr. Khan delivered a very fruitful lecture talk on “OMICS to Systems Biology: A way to address health challenges” on National training workshop and highlighted the importance of throughput genomics of microbial genome. He described briefly about the mechanism of drug resistance and target identification for various diseases by using different systems biology approaches.

He described about the era of proteomics and suggested that it is the next step in the study of biological systems. It is more complicated than genomics because an organism's genome is more or less constant, whereas the proteome differs from cell to cell as well as time to time. Distinct genes are expressed in different cell types, which mean that even the basic set of proteins that are produced in a cell needs to be identified. The proteome is the entire set of proteins that are produced or modified by an organism or system. Proteomics has enabled the identification of ever increasing numbers of protein. Proteomics confirms the presence of the protein and provides a direct measure of the quantity present. System biology based approach has been emerged as a most decent approach to investigate the target protein to its functional or phenotypic level. Systems biology is the computational and mathematical modeling of complex biological systems. It is a biology-based interdisciplinary field of study that focuses on complex interactions within biological systems, using a holistic approach to biological research. Systems biology has been responsible for some of the most important developments in the science of human health and environmental sustainability. It is a holistic approach to deciphering the complexity of biological systems that starts from the understanding that the networks that form the whole of living organisms are more than the sum of their parts. It is collaborative, integrating many scientific disciplines – biology, computer science, engineering, bioinformatics, physics and others – to predict how these systems change over time and under varying conditions, and to develop solutions to the world's most pressing health and environmental issues. Network-based approaches for analyzing high dimensional genomic data sets

such as; weighted correlation network analysis is often used for identifying clusters, modeling the relationship between clusters, calculating fuzzy measures of cluster (module) membership, identifying intra-modular hubs, and for studying cluster preservation in other data sets. Pathway-based methods for omics data analysis and these approaches have to identify and score pathways with differential activity of their gene, protein, or metabolite members. (Figure 1)

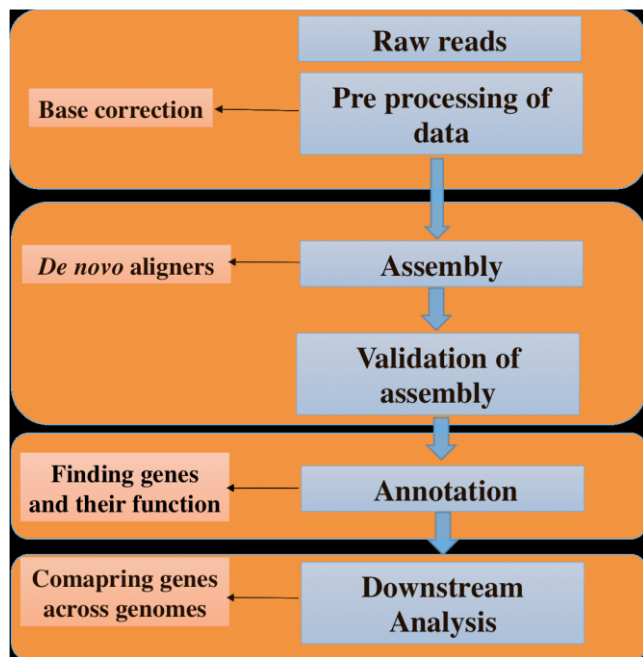
In the afternoon session Dr. Anil Kumar, Director Education, RLBCAU, Jhansi presented a very informative lecture related to “Hi-throughput Omics data analysis by utilizing the power of Bioinformatics and Systems Biology Tools” and provided a fundamental concepts of Omics technology, computational tools for experimentation and interpretation of the biological data in context of plant biology. Dr. Kumar discussed about key concepts of Omics for better understanding of biological systems with respect to biotechnological research for improving agricultural productivity.

In the evening session, Professor Dr. Sandeep Arora and Research Staff of the Department including Dr. Supriya Gupta, Dr. Aparna Agrawal, and Ms. Darshana demonstrated the various instruments of Bio Safety, Proteomics, Cytogenetics and Plant Stress & Molecular Cell biology lab and its application in Systems Biology. Later Mr. Apoorv Tiwari, SRF and Mr. Rutash Kumar, JRF in the Centre performed a practical module on “Bioinformatics Basics” and describe about different file formats of nucleotide and protein sequences and Structures and also describe about different functions of command prompt.

In the 2<sup>nd</sup> day of workshop, Dr. Atul Kumar, Professor, Plant Physiology, CBSH, GBPUA&T, Pantnagar presented an informative lecture talk on “A Journey from Plant Physiology to Systems Biology”. Dr. Kumar describe that the systems biology and present scenario, expanding our understanding for a holistic view of the functions and forms of biological systems as an iterative process is the main objective of research on Systems Biology. In the present scenario, expanding our understanding for a holistic view of the functions and forms of biological systems as an iterative process is the main objective of research on Systems Biology. Plant Physiologists and Ecologists have already been using a systems approach to study plants for many years; a systems biology approach dealing with molecular details looks feasible now with the advent of genomic technologies. For the first time, this has opened exciting prospect of the post-genomic era to integrate knowledge across different levels of biological organization and to anchor this at the molecular level. Plants, however, pose additional aspects of biological complexity including numerous organelles, tissues, organs and genome complexity (e.g., ploidy levels). He suggest to develop an *in silico* model of the plant that encompasses all levels of biological organization (molecular, cellular, physiological, and ecological).

Dr. Atul Upadhyay, Assistant Professor, Lovely Professional University, Jalandhar, Punjab delivered a lecture talk on Next Generation Sequencing: Data analysis and applications" and described that Genomics, the word itself drags our consciousness toward its Greek origin “genesis” meaning a body of gene and the word “omics” meaning the study of a field. Genomics means the branch of molecular biology concerned with the structure, function, evolution, and mapping of genomes. Genome includes the complete set of DNA content present within an organism. He also presented a hands-on module on "Genome sequence databases and their role in data analysis. During hand-on module Dr. Atul

elaborated the Major steps of NGS data analysis which are Pre-assembly, denovo and reference based assembly and annotation of assembled genome (Figure 2).



**Fig 2:** Major steps of a typical NGS data analysis. Starting from pre-processing of raw reads before assembly followed by genome annotation and downstream analysis.

Later, Mr. Apoorv Tiwari, SRF, Sub-DIC Bioinformatics, delivered a Hands-on module on “Transcriptome/Genome/Proteome Sequence homology search Using Standalone BLAST” and described about the importance of Standalone blast for sequence analysis. Mr. Apoorv Tiwari and Mr. Rutash Kumar performed practical module on Basic local alignment of high-throughput sequencing data for mining of important genes/proteins linked with specific traits.

In the 3<sup>rd</sup> day of workshop a very informative lecture Talk delivered by Dr. S.D. Samantaray, Professor, College of Technology, GBPUA&T, Pantnagar on “Pattern Mining Approaches” briefly described about the different algorithms and computational languages widely used in systems biology. He also described about different approaches for mining of biological data and solves biological problems using perl scripting language.

After that Mr. Neetesh Bandhiwal, Bioinformatics Team Head, NxGenBio Life Sciences Pvt. Ltd., New Delhi delivered a lecture talk on “Data analyzing and associating traits with regions of genome by Genotyping by Sequencing (GBS)” and also performed a hands on module on “GBS Data analysis”. He described the exponential reduction in sequencing costs with advances in Next Generation Sequencing (NGS) technologies has led to rapid developments in the field of genotyping technologies. Genome complexity reduction methods such as Restriction Associated DNA sequencing (RAD-seq) and Genotyping by sequencing (GBS) has emerged as powerful genotyping platform which are capable of discovering, sequencing and genotyping not hundreds but thousands of markers across almost any genome of interest, but also number of individuals in a population in a single and simple experiment. GBS currently usage low coverage sequencing protocol backed by power of NGS for genotyping large populations and more precise association of genotype and phenotype. Few potential drawbacks of GBS are large proportion of missing data points due to low coverage of

sequencing, management and analysis of large amount of sequence data. But with further increase in sequencing output, availability of more reference genomes and developments in field of bioinformatics will further empower these techniques. However flexible, rapid and low cost of GBS makes it an excellent tool for many applications and to address many questions of plant breeding and genetics. This review summarizes the family of GBS approaches and its potential to hold a genome wide genotyping platform.

Later Dr. Dev Bukhsh Singh, Assistant Professor, Department of Biotechnology, CSJM University, Kanpur delivered a very informative lecture Talk on “Principles and Approaches for 3D structure Modeling and Validation” and discussed various computational biology approaches modeling of tertiary structure of proteins and their role in medical sciences. Dr. Singh described about the algorithms and software’s for protein structure modeling and validation. He also described in detail about the protein folding and its prediction of (tertiary, 3-dimensional) protein structure given the (primary, linear) structure defined by the sequence of amino acids of the protein. He told that the experimental approaches for protein structure prediction like X- Ray Crystallography and Nuclear magnetic resonance are too costly and time taking but by the use of computational approaches it makes easy, with no cost and time. After that Mr. Rutash Kumar (JRF) and Mr. Apoorv Tiwari (SRF) performed Hands on Module on “Molecular Structure Prediction and described different steps for protein structure prediction and validation through MODELLER.

In 4<sup>th</sup> day of the workshop, Dr. Dev Buksh Singh, presented another lecture on “Natural Product and optimization strategies to achieve better potency”. He described that molecular docking has become an increasingly important tool for drug discovery. He covered the brief introduction of the available molecular docking methods, and their development and applications in drug discovery. Natural products can be used as resource for new drugs. Nature provides a boundless set of structurally diverse compounds that can be used as a medicine. Natural products have made immense contribution to drug discovery over the many decades and remain an important source of structural and molecular diversity for drug discovery. Large number of natural products may serve as important leads for further drug development in many diseases. Later Mr. Rutash Kumar and Mr. Apoorv Tiwari performed Hands on Module on “Molecular Docking”.

The last lecture on “RNA seq Analysis and Algorithms” presented by Dr. Soma S Marla, Principal Scientist, NIPGR, New Delhi. He described that RNA- seq is an important transcriptome analysis technique for characterization and understanding of variation in biology existing at molecular level. Cells during growth and development dynamically access information from genome and translate specific instructions through ‘gene expression’ by selectively switching on and off of a particular set of genes. Thus, the set of RNAs transcribed in a certain condition (for example during a disease) and time reflects the current state of a cell and can reveal plant response during pathogenesis. Interestingly, comparative study of gene expression profiles of diseased vs. healthy plants enables to identify genes that play a major role. He suggests some popular tools (available in public domain) for mapping on to reference genome and alignment including BOWTIE, TOPHAT, BFAST, MAQ, SHRIMP and SOAP etc.

In the 4 days national training workshop a total of 9 lectures with practical modules were covered to provide directional

flow of information in agricultural sciences to 22 participants of different states (Figure 3).



**Fig 3:** Group photograph of scientists, research scholars and academic staff during workshop valedictory function

### Feedback analysis and conclusions

With response to our publicity we tend to received several applications from throughout the country. Twenty two participants were selected based on 1st come 1st serve basis. The workshop drew 22 participants representing academia, industry, and research organizations across India. Participants' feedback was also asked to judge the end result of the workshop. The feedback consisted of sub-domains, starting from technical experience to learning expertise to active coaching to cordial reception rendered. The domains included as overall workshop assessment; talks on bioinformatics, systems biology; technical acumen of trainers; active training; workshop hand-outs; workshop conduct; logistics; outcome evaluation; enhancements for future workshops and overall impressions, comments, and suggestions. The organizers were gratified by participants' self-analysis of their knowledge, skills, and confidence with respect to combining laboratory exercises with the use of different systems biology during the workshop. Thus, it was absolutely clear from the feedback analysis that the workshop was a substantial success.

Gradual increase in the high-quality hi-throughput data and mathematical modeling of biological processes by using different bioinformatics tools will lead to better strategies to researchers for development of crop varieties for robust agricultural productivity and sustainability. Efforts made toward enhancing our knowledge base and broadening our knowledge towards Omics and Systems biology is ultimately aimed at improving our academic standards and its use in the welfare of our society. In these efforts, our knowledge partner Nx Gen Bio Life sciences Pvt. Ltd. New Delhi was also involved in providing valuable knowledge and tools for the benefits of our participants. The Organizer of the workshop Dr. Gohar Taj devoted her sincere thanks to Dean CBSH Dr. A.K. Shukla, for his valuable guidance, Dr. Anil Kumar Gaur, Head MBGE and all the teaching and non teaching staff for successful completion of the workshop.

### Acknowledgements

Authors are grateful to Biotechnology Information System Network (BTIS Net), Department of Biotechnology, Government of India, New Delhi for providing financial assistance to Bioinformatics Sub DIC for conducting quality teaching, training, and research in emerging area of Bioinformatics at Pantnagar.

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