Department of Applied Sciences

Coursework Structure and Syllabus of Ph. D. Program

PROGRAM OBJECTIVES:

- To prepare quality doctorates knowledgeable in their respective research domain.

PROGRAM OUTCOMES:

- Graduates of this program will demonstrate the necessary skills to become productive, ethical,and independent scientists.
- Graduates will understand and critically evaluate current research in their chosen area of research.
- Graduates will learn the basic pre-requisites to identify new research problems in respectivedomain.

<u>Course Structure of Ph. D. in Applied Mathematics</u>
(Approved by AC.40/2021/2/3.5, AC.43/2022/2/3.1)

A student must complete minimum 16 credits including 'Doctoral Research Methodology' in the Department of Computer Science & Engineering (CS 704) and 'Ethics in Research' as the compulsory courses. The rest of the credits can be earned by completing at least one course from the Department of Applied Sciences, and Open Elective/ MOOCs.

Course Code	Course Name	L-T-P	CH	Credit	Remarks
CS 704	Doctoral Research Methodology	4-0-0	4	4	Offered by the Department of Computer Science & Engineering
RP 799	Research and Publication Ethics	2-0-0	2	2	Offered by the School of Engineering
XXXX	MOOCs/ Open Elective	x-x-x	x	3/4	Online platforms or courses offered by other departments
AM 701	Inventory Modeling	3-1-0	4	4	Offered by the Department of Applied Sciences
AM 702	Optimization Techniques	3-1-0	4	4	Offered by the Department of Applied Sciences
AM 703	Transportation Problems and Soft Computing	3-1-0	4	4	Offered by the Department of Applied Sciences
AM 704	Graphs and Matrices	2-2-0	4	4	Offered by the Department of Applied Sciences
AM 705	Linear Algebra and Applicable Matrix Theory	2-2-0	4	4	Offered by the Department of Applied Sciences
AM706	Topics in Fourier analysis	3-1-0	4	4	Offered by the Department of Applied Sciences (Approved by AC.42/2022/2/3.5)
AM707	Topics in Theory of Partial Differential Equations	3-1-0	4		Offered by the Department of Applied Sciences (Approved by AC.42/2022/2/2.5)

AM 701: Inventory Modeling **L-T-P-Cr-CH: 3-1-0-4-4**

Course Outcomes:
On successful completion of the course, the student will:

CO1. Identify and develop inventory models from the verbal description of the real system.
CO2. Analyze any real-life system with limited constraints and depict it in a model form.
CO3. Apply different mathematical techniques constructively to make effective business decisions.
CO4. Be able to understand the characteristics of different types of decision-making environments and the appropriate decision-making approaches and tools to be used in each type of model.

Course Contents:

Unit 1: Understanding the Supply Chain.
Introduction on the objective of a Supply Chain, The importance of Supply Chain in decisions, Decisionphases in a Supply Chain, Process views of a Supply Chain, Examples of Supply Chains.

Unit 2: Stocks and Inventories
Stocks of materials, Reasons for holding stocks, Stocks in the supply chain, Approaches to inventorycontrol, Factors involved in inventory problem analysis.

Unit 3: Inventory Model Building
Steps of inventory model building, Replenishment order size decisions and concepts of EOQ, EPQ models, Classification of EOQ models and EPQ models, Uncertainty in demand and costs, Lead time, Reorder point.

Unit 4: Deterministic Inventory Control Models
Single items inventory control models with and without shortages, Single item inventory control models with quantity discounts, Multi item inventory models with constraints, Inventory control models with uncertain demands, Inventory control models with deterioration.

Unit 5: Probabilistic Inventory Control Models
Instantaneous demand inventory control models with and without set-up cost, Continuous demand inventory control models without set-up cost.

Unit 6: Reorder point, Lot size models: The Continuous Review Case
An approximate model when backordering is permitted, An exact model for determining the stationary distribution of the inventory position random variable, An exact model for determining the stationary distribution of the net inventory random variable

Textbooks:

1. Principles of Inventory Management: When You are Down to Four, Order More. J. Muckstadt,and A. Sapra, Springer, 2010.
2. Operations Research: Theory & Applications, J.K. Sharma, Macmillan India Ltd., Third Edition,2007

References:

1. Supply Chain Management: Strategy, Planning, and Operation, S. Chopra and P. Meindl,Pearson, Fifth Edition, 2016
2. Operations Research, R. Panneerselvam, PHI Learning Private Limited, Second edition, 2019.
3. Operations Research, P.K. Gupta and D.S. Hira, S. Chand, Seventh Edition, 1976

AM 702: Optimization Techniques **L-T-P-Cr-CH:3-1-0-4-4**

Course Outcomes:
On successful completion of the course, the student will:

CO1. Be able to model mathematical minima/maxima problems as optimization problems.
CO2. Be able to determine maximization and minimization of convex functions.
CO3. Solve nonlinear problems through its linear approximation.
CO4. Solve different types of programming problems and apply on solving multi-objective problems.
CO5. Apply various types of direct and gradient-based search methods.

Course Contents:

Prerequisite: Definition and importance of optimization, Basic terminologies, General problem formulation, Local and global optimum, Concave and convex functions.

Unit 1: Single variable linear and non-linear unconstrained optimization – first and second order optimality criteria, Bracketing and refining optimum point, Direct search methods, Gradient-based search methods; Multi-variable linear and non-linear unconstrained optimization - first and second order optimality criteria, Unidirectional search, Direct search methods, Gradient-based search methods.

Unit 2: Constrained linear programming problems – simplex method, Duality in linear programming, Constrained extremal problems; Constrained nonlinear programming problems - Kuhn-Tucker conditions, sensitivity analysis, Penalty function methods, Method of multipliers, Direct search methods, Sequentially linearized methods, Feasible direction method, Gradient-based search methods.

Unit 3: Quadratic programming; Convex programming, Non-convex programming, Goal programming, Robust Optimization, Fuzzy programming technique, Interactive fuzzy decision-making method, Weighted sum method, Chance constrained optimization techniques.

Unit 4: Specialized algorithms for integer and geometric programming problems; Application of differentoptimization methods to operations research problems.

Textbooks:

1. Optimization for Engineering Design – Algorithms and Examples, K. Deb, Prentice-Hall

of India,Third edition, 1995
2. Introduction to Optimum Design, J.S. Arora, Academic Press, 2004

References:

1. Optimization Concepts and Applications in Engineering, A.D. Belegundu and T.R. Chandrupatla,Pearson Education, 1999
2. Optimization: Theory and Applications, S.S. Rao, Wiley Eastern, 1984

AM 703: Transportation Problems and Soft Computing L-T-P-Cr-CH: 3-1-0-4-4

Course Outcomes:
On successful completion of the course, the student will:

CO1. Be able to formulate different types of transportation and linear programming models.
CO2. Be able to solve new research applications of linear programming problems.
CO3. Analyze new multi-variable, multi-index, multi-objective transportation problems.
CO4. Be able to apply soft computing techniques to solve multi-objective transportation problems.
CO5. Be able to design different types of disaster transportation models.

Course Contents:

Unit 1: Linear Programming Problems
Single and multi-dimensional constrained LPP, Single and multi-dimensional unconstrained LPP, Linear programming under uncertainty, Minimal-cost network flows, LPP with interval coefficients. Integer linear programming, Standard applications of linear programming.

Unit 2: Transportation Problems (TPs)
Multi-variable TPs, Multi-index TPs, Multi-objective TPs, TP in crisp and fuzzy environment, TP in probabilistic environment, Multi-objective transportation problem (MOTP) and different approaches to solve MOTP, Transportation problem with interval coefficients and their different solution techniques. Transportation problem with different types of variable cost and constraint and their solutions.

Unit 3: Disaster Transportation Models:
Emergency resource management in disaster: certain and uncertain environment, Involvement of NGO in relief operation, Implementation of Transportation models in disaster within various environment, Importance of social media in relief operation, Impact of debris on resource management and its cleaning plan.

Unit 4: Soft Computing
Introduction of soft computing, Fuzzy logic, Genetic Algorithm, Neural networks, Application of fuzzy logic concepts in scientific problems, Solution of optimization problems using Genetic Algorithm. Neural

Network approaches in scientific analysis, Design and diagnostic problems. Multi-objective optimizationproblem (MOOP) definition, Understanding the concept of compromise solutions for MOOP.

Unit 5: Programming Language
Programming with C, C++, C-plex, Software Packages: LINGO, EXCEL, MATLAB

Textbooks:

1. Operations Research: Principles and Application, G. Srinivasan, Prentice-Hall of India, 2010
2. Artificial Intelligence and Soft Computing for Beginners, A. Das., Arizona Business Alliance,2014

References:

1. Soft Computing: With Matlab Programming, N.P. Padhy and S.P. Simon, Oxford UniversityPress (OUP), 2015
2. Handbook of research on the applications of international transportation and logistics for worldtrade, G. C. Ceyhun. Hershey, PA : Business Science Reference, 2020

AM 704: Graphs and Matrices **L-T-P-Cr-CH: 3-1-0-4-4**

Prerequisites: Discrete Mathematics
Course Outcome:
On successful completion of the course, the student will:

CO1. Be able to create the required foundation for solving research problems in the domain of spectralgraph theory.
CO2. Be able to identify the use of advanced matrix theory to characterize a graph and its severalvariations in general.
CO3. Be able to understand the interlink between graph and various associated matrices.
CO4. Be able to demonstrate the use of eigenvalues of a matrix that characterizes a graph and vice versa.
CO5. Be able to apply the knowledge of some already done research problems to tackle new problems.

Course Contents:

Unit 1: Preliminaries: -Matrices, Eigenvalues of symmetric matrices, Generalized inverses.

Unit 2: Incidence Matrix: - Rank, Minors, Path matrix, Moore–Penrose inverse, 0-1 Incidence matrix.

Unit 3: Adjacency Matrix: - Eigenvalues of some graphs, Determinant, Spectral radius, Energy of agraph, Nonsingular trees.

Unit 4: Laplacian Matrix: - Basic properties, Computing Laplacian eigenvalues, Matrix-tree theorem,Laplacian spectral radius, Edge–Laplacian of a tree.

Unit 5: Algebraic Connectivity: - Preliminary results, Classification of trees, Monotonicity properties ofFiedler vector, Bounds for algebraic connectivity.

Unit 6: Distance Matrix: - Distance matrix of a graph, Distance matrix and Laplacian of a tree, Eigenvalues of the distance matrix of a tree.

Unit 7: Resistance Distance: - The triangle inequality, Network flows, A random walk on graphs,Effective resistance in electrical networks, Resistance matrix.

Textbooks:
1. Graphs and Matrices, R.B. Bapat, Springer and Hindustan Book Agency, New Delhi, 2010.
2. Spectra of Graphs, A. E. Brouwer and W.H. Haemers, Springer, 2012.

3. Algebraic Graph Theory, C. Godsil and G.F. Royle, Springer, 2001.
4. Matrix Analysis, R. Horn and C.R. Johnson, Cambridge University Press, 1985.
5. Graph Theory with Applications to Engineering and Computer Science, N. Deo, DoverPublications, Inc. 2016.

References:

1. Graph Theory with Applications, J.A. Bondy and U.S.R. Murthy, Macmillan Press, 1976.
2. Topics in Matrix Analysis, R. Horn and C.R. Johnson, Cambridge University Press, 1999(Reprint).

AM 705: Linear Algebra and Applicable Matrix Theory L-T-P-Cr-CH: 3-1-0-4-4

Prerequisites: MS 403 Linear Algebra

Course Outcome:
On successful completion of the course, the student will:

CO1. Be able to create the required foundation for solving research problems in the domain of spectralgraph theory.
CO2. Be able to identify the use of advanced matrix theory that is used to solve problems of spectralgraph theory.
CO3. Be able to use the various factorization and canonical forms of a matrix for specific problem athand.
CO4. Be able to apply the knowledge of various kinds of generalized inverses of a matrix.

Course Contents:

Unit 1: Unitary matrices, Normal matrices, Hermitian and skew Hermitian matrices, variational characterization of eigenvalues.

Unit 2: Positive definite matrices, Positive semidefinite matrices.

Unit 3: General Matrices: The matrices AA^T and A^TA, Singular Values, Singular Value Decomposition.
Unit 4: Canonical factorization, Q-forms.
Unit 5: Courant-Fischer minmax & related theorems. Perron-Frobenius theory.
Unit 6: Nonnegative matrices, positive matrices, Irreducible matrices, Reducible matrices.

Textbooks:

1. Matrix Analysis, R. Horn and C.R. Johnson, Cambridge University Press, 1985.
2. Matrix and Linear Algebra, K.B. Datta, PHI, 1991.
3. Nonnegative Matrices, H. Minc, John Wiley and Sons, 1988.

References:

1. Nonnegative Matrices and Applications, R.B. Bapat and T.E.S. Raghavan, Cambridge UniversityPress, 1997.
2. Nonnegative Matrices in the Mathematical Sciences, A. Berman and R.J. Plemmons, AcademicPress, 1979.

AM 706 Topics in Fourier Analysis **L-T-P-Cr-CH:3-1-0-4-4**

Prerequisites: Nil

Course Outcome:

On successful completion of the course, the student will:

CO1. Be able to compute and prove the convergence of Fourier series.

CO2. Be familiar with the modern theory of Fourier Analysis

CO3. Be able to apply the knowledge of Fourier transform in Hilbert transform and similar singular integrals

Course contents:

Unit 1

Basics of Fourier series, Plancherel theorem for Fourier Series, harmonic functions in the unit disc, Poisson integrals, Poisson theorem.

Unit 2

Various means of convergence of Fourier Series.

Unit 3

Conjugate Fourier Series, Hilbert transform on the circle and its properties.

Unit 4

Fourier transform of L^1, L^2 and L^p , $1<p< 2$ functions, Properties of Fourier transform.

Unit 5

Test functions, Distributions, Tempered distributions, Fourier transform of L^p, $p>2$ functions.

Unit 6

Approximations to the identity, Hardy-Littlewood Maximal Function and boundedness, Lebesgue differentiation theorem, Dyadic Maximal function, and its boundedness.

Unit 7

Hilbert transform and its boundedness.

Textbook:

1. Pinsky, M. A., *Introduction to Fourier Analysis and Wavelets,* Graduate Studies in Mathematics, Vo. 102, AMS, 2001

References:

1. Bhatia, R., *Fourier Series*, Texts and Readings in Mathematics, Vol. 2, Hindustan Book Agency, New Delhi
2. Stein, E. M. and Shakarchi, R. *Functional Analysis*, Princeton Lect. In AnalysisVol-4, 2011
3. Stein, E. M. and Weiss, G. *Introduction to Fourier Analysis in Euclidean Spaces*, Princeton University Press, Princeton, 1971.
4. Katznelson, Y. *An Introduction to Harmonic Analysis*, Cambridge Mathematical Library, Reprint 2004.
5. Chandrasekharan, K. *Classical Fourier Transform*, Universitext, Springer Verlag, 172, 1989.
6. Grafakos, L. *Classical Fourier Analysis*, Graduate Text in Mathematics, Springer, 249, 2009
7. Grafakos, L. *Modern Fourier Analysis*, Graduate Text in Mathematics, Springer, 250, 2009

AM 707 Topics in Theory of Partial Differential Equations L-T-P-Cr-CH:3-1-0-4-4

Prerequisites: Nil

Course Objectives:

On completion of the course, the student will:

CO1. Be familiar with the modern theory of partial differential equations.

CO2. Be able to study and construct the weak solutions of boundary value problems.

CO3. Be able to apply the knowledge of the course to research problem in the theory of partial differential equations.

Course contents:

Unit -1

Review of Lebesgue measure, measurable functions, Lebesgue integration, Product measures and Fubini's theorem, differentiability of functions, absolutely continuous functions, Lp spaces.

Unit -2

Change of variable and integration by parts in R^n, Test functions and distribution, tempered distribution, the Fourier transform, the inverse Fourier transform.

Unit -3

Sobolev spaces, extension theorems, embedding theorems, compactness theorem, inclusion relations and Sobolev's inequality, negative norms and duality, fractional order Sobolev space, trace theorems for all $1 \leq p < \infty$.

Unit -4

Variational formulations of elliptic boundary value problems, Lax-Milgram principle, regularity of weak solutions, eigen value problems, Galerkin method.

Textbook:

2. Kesavan, S., *Topics in Functional Analysis and Applications*, New Age International(P) Limited Publishers, 1989

References:

8. Royden, H. L., *Real Analysis*, Pearson Education India, 1968 (reprint in 2015).
9. Evans, L. C., *Partial Differential Equations*, Graduate Studies in Mathematics, Vol. 19, AMS, 1988.
10. Renerdy, M. and Rogers, R. C., *An Introduction to Partial Differential Equations*, Text in Applied Mathematics, Springer, Vol 13, 1993.
11. Taylor, M. E., *Partial Differential Equations* I, II, III, Applied Mathematical Sciences,Vol. 115-117, Springer, 1998.

Course Structure of Ph. D. in Applied Chemistry
(Approved by AC.40/2021/2/3.5, AC.43/2022/2/3.1)

A student must complete minimum 16 credits including 'Doctoral Research Methodology' in the Department of Computer Science & Engineering (CS 704) and 'Ethics in Research' as the compulsory courses. The rest of the credits can be earned by completing at least one course from the Department of Applied Sciences, and courses from Department of Chemical Sciences, or Open Elective, or MOOCs.

Course Code	Course Name	L-T-P	Course Hours	Credit	Remarks
CS 704	Doctoral Research Methodology	4-0-0	4	4	Offered by the Department of Chemical Sciences
RP 799	Research and Publication Ethics	2-0-0	2	2	Offered by the Department of Chemical Sciences
XXXX	Open Elective, MOOCs, etc.	x-x-x	x	3/4	Offered by the Department of Chemical Sciences
AC 701	Supramolecular Chemistry	4-0-0	4	4	Offered by the Department of Applied Sciences
AC 702	Chemistry of Porous Materials	4-0-0	4	4	Offered by the Department of Applied Sciences
CH-713	Applications of Spectroscopic Tools	3-1-0	4	4	Offered by the Department of Chemical Sciences
CH-715	Advanced Instrumental Methods in Chemistry	2-0-2	6	4	Offered by the Department of Chemical Sciences
CH-716	Green Chemistry	2-2-0	4	4	Offered by the Department of Chemical Sciences
CH-722	Polymeric Nanocomposites	3-1-0	4	4	Offered by the Department of Chemical Sciences
CH-723	High Performance Polymers	3-1-0	4	4	Offered by the Department of

					Chemical Sciences
CH-725	Catalytic Chemistry	3-1-0	4	4	Offered by the Department of Chemical Sciences
AC601	Introduction to Polymer Science	3-1-0	4	4	Approved by AC.43/2022/2/2.5
AC602	Analytical Techniques in Polymer Chemistry	3-1-0	4	4	Approved by AC.43/2022/2/2.5

AC 701: Supramolecular Chemistry **L-T-P-CR-CH: 4-0-0-4-4**

Course Outcomes:

CO1. In this course, the students will learn different aspects of supramolecular chemistry and nanoscience.

CO2. They will learn about different types of crystalline (molecular and polymeric) solid materials, their structural features and properties, crystal engineering approaches to modulate the properties and their potential applications.

CO3. The students will learn scientific writing and research presentations through assignments on writing research proposals, reviews etc. and short class presentations on state-of-the-art research topics within the scope of the course. These will familiarize them with some of the cutting-edge research areas of chemistry.

Course Contents:

Unit 1: Different types of supramolecular interactions
ionic interactions, ion-dipole interactions, dipole-dipole interactions, ion-induced dipole and dipole- induced dipole interactions van der Waals or dispersion interactions, hydrogen bonding, halogen bonding,anion-pi interactions, pi-pi interactions, aromatic-aromatic interactions.

Unit 2: Molecular recognition
molecular receptors for neutral and charged guests, cation and anion binding hosts, podands, macrocycles, crown ethers, cryptands, cavitands, spherands, cucurbiturils, cyclodextrins, catenanes, rotaxanes, molecular knots, intercalates, molecular recognition at the air-water interface, Langmuir-Blodgettry

Unit 3: Solid-state chemistry of organic molecules
crystal growth, molecular packing in crystals, polymorphs, solvates, co-crystals, salts, solid solutions, amorphous solid forms, phase transformations.

Unit 4: Crystal engineering
supramolecular synthons, structure-property correlation in crystalline solids, design of crystalline solids with targeted properties

Unit 5: Network solids
hydrogen-bonded organic frameworks (HOFs), coordination polymers (CPs), metal-organic frameworks (MOFs), covalent-organic frameworks, polymers of intrinsic microporosities (PIMs)

Unit 6: Applications:

biomimetic systems with ion transport properties, sensors materials, molecular machines, stimuli responsive crystalline solids, porous solids with chemical separation and storage properties, nanoengineering of electronic devices, etc.

Text Books:

1. Supramolecular Chemistry: Concepts and Perspectives. J.-M. Lehn, Wiley-VCH Verlag GmbH,1995.
2. Principles and Methods in Supramolecular Chemistry. H. J. Schneider and A. Yatsimirsky,Wiley, New York, 1999.
3. Supramolecular Chemistry. J. W. Steed and J. L. Atwood, John Wiley & Sons, Chichester, 2009.

References:

1. Crystal Engineering: The Design of Organic Solids. G.R. Desiraju, Elsevier, 1989.

AC 702: Chemistry of Porous Materials L-T-P-CR-CH: 4-0-0-4-4

Course Outcomes:

CO1. In this course, the students will be familiarized with the chemistry in the nano-space.
CO2. They will learn about different types of crystalline and amorphous poroussolid materials, theirstructural features, and properties, approaches to modulate the properties and their potential applications. **CO3.** The students will learn scientific writing and research presentations through assignments on writing research proposals, reviews etc. and short class presentations on state-of-the-art research topics within the scope of the course. These will familiarize them with some of the cutting-edge research areas ofchemistry.

Course Contents:

Unit 1: Introduction to porous materials, their characteristics features, techniques of characterization,basic principles of gas sorption, determination of materials porosity.

Unit 2: Small molecular systems with intrinsic porosities, molecular containers, supramolecularinteractions and host-guest chemistry, chemical reactions in confined space

Unit 3: Inorganic porous materials: activated carbon, mesoporous silica, zeolites, etc.; their syntheses andproperties

Unit 4: Different types of crystalline and amorphous porous organic polymers (POPs): polymers of intrinsic microporosity (PIMs), conjugated microporous polymers, porous aromatic frameworks (PAFs), cross-linked polymers, covalent organic frameworks (COFs), etc.

Unit 5: Coordination polymers (CPs), metal-organic frameworks (MOFs) zeolitic imidazolate frameworks, different types of hybrid porous materials, post-synthetic modifications

Unit 6: Hydrogen-bonded frameworks (HOFs) and other supramolecular frameworks: design principlesto access porosity and properties of these materials.

Unit 7: Potential applications of porous materials in heterogeneous catalysis, membrane-based separation, gas storage, targeted chemical delivery, sensing, electronic devices, etc., approaches to tailor their properties for targeted applications.

Unit 8: Comparative studies among different types of porous materials, opportunities and challenges withthese materials, recent developments, and future prospects

Text Books:

1. Porous Polymers: Design, Synthesis and Applications. Shilun Qiu and Teng Ben, Royal Societyof Chemistry, 2016. https://doi.org/10.1039/9781782622260
2. The Chemistry of Metal–Organic Frameworks: Synthesis, Characterization, and Applications,Volume 1. Stefan Kaskel, Wiley-VCH Verlag GmbH & Co. KGaA, 2016.

References:

1. Themed collection on Molecular Containers in Chemical Society Reviews, 2015. https://pubs.rsc.org/en/journals/articlecollectionlanding?sercode=cs&themeid=8125df83-c480- 4256-9a87-5a14078fb2d0

2. Introduction to Reticular Chemistry: Metal-Organic Frameworks and Covalent Organic Frameworks.
3. Omar M. Yaghi Markus J. Kalmutzki Christian S. Diercks, Wiley-VCH Verlag GmbH & Co. KGaA, 2019. https://onlinelibrary.wiley.com/doi/book/10.1002/9783527821099

4. Hydrogen-Bonded Organic Frameworks: A Rising Class of Porous Molecular Materials.
5. Penghao Li Matthew R. Ryder and J. Fraser Stoddart, *Acc. Mater. Res.***2020**, *1*, 77–87.https://doi.org/10.1021/accountsmr.0c00019

AC-601 Introduction to Polymer Science L-T-P-**Cr** 3-1-0-**4**

Course Outcomes:

On completion of this course, students will be able to:

CO1: Learn about the basics of polymers, polymerization methods and techniques

CO2: Know the methods of characterization and processing of polymers

CO3: Understand the structure-property relationship in polymer

Course Contents:

Unit 1: Introduction to Polymers [06 Lectures]

Importance, raw materials, basic nature and classification of polymers. Average molecular weight and molecular weight distribution. Polymerization Methods and Techniques, Types of copolymers: Random, Block and graft copolymers.

Unit 2: Characterization Methods [8 Lectures]

Chromatographic method, Spectroscopic methods, X-ray diffraction study, microscopy, thermal analysis, and thermal transition in the polymer (Tg, Tm). Physical testing: tensile strength, tear strength, fatigue failure, resilience, hardness, impact and abrasion resistance.

Unit 3: Structure and Properties [8 Lectures]

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Concept of solubility parameter and its application.

Polymer structure and physical properties-crystalline melting point Tm - melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion.

The glass transition temperature Tg: Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking.

Unit 4: Rheology and Processing Techniques [06 Lectures]

Basic Introduction to Rheology: Viscoelasticity, Newtonian, Non-Newtonian fluids, Compounding and reinforcing, Processing techniques: two-roll mill mixing, internal mixer, calendaring, film casting, moulding, extrusion and fibre spinning.

Unit 5: Polymer Blend and Nanocomposites [4 lectures]

Preparation, Types of blends, types of nanofillers, Thermodynamical considerations, Property enhancements, Application of blends and nanocomposites

Unit 6: Application of Synthetic Polymers [4 lectures]

Materials and Biological importance. Nanomaterials, Conducting polymers, Polymers for renewable energy. Polymers for advanced materials

Recommended Books:

1. Carraher Jr, C. E. (2017). *Introduction to polymer chemistry*. CRC press.
2. Peacock, A. J., & Calhoun, A. (2012). *Polymer chemistry: Properties and application*. Carl Hanser Verlag GmbH Co KG.
3. Gowariker, V. R., Viswanathan, N. V., & Sreedhar, J. (2019). *Polymer science*. *Third edition*. New Age International.
4. Fried, J. R. (2014). *Polymer science and technology*. Pearson Education.
5. Youssef, G. (2021). *Applied mechanics of polymers: properties, processing, and behavior*. Elsevier.
6. Puskas, J. E. (2013). *Introduction to polymer chemistry: A biobased approach*. DEStech Publications, Inc.
7. Odian, G. (2004). *Principles of polymerization*. John Wiley & Sons.
8. Sperling, L. H. (2005). *Introduction to physical polymer science*. John Wiley & Sons.

AC - 602 Techniques in Polymer Chemistry L-T-P-**Cr** 3-1-0-**4**

Course Outcomes:

On completion of this course, students will be able to:

CO1: Learn about various analytical techniques used for the identification and structural evaluation of polymeric materials

CO2: Understand the use of various microscopy techniques for morphological studies.

CO3: Learn the use of DSC and TGA for the evaluation of thermal properties

Course Contents:

Unit 1: Spectroscopic and Diffraction Methods

General principles, instrumentation and applications of the following spectroscopic and diffraction techniques.

For structural analysis: UV/Visible Spectroscopy, Infrared Spectroscopy (IR) and Nuclear Magnetic Spectroscopy (NMR)

For surface analysis: X-Ray Photoelectron Spectroscopy (XPS) and Time-of-Flight Secondary Ion Mass Spectrometry (*TOF-SIMS*)

For bulk analysis: X-ray diffraction (XRD) technique.

Unit 2: Microscopic Techniques

Working Principle, instrumentation and applications of Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and Contact Angle Measurements.

Unit 3: Thermal Analysis

Principles, instrumentation and applications of Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (DTA).

Unit 4: Chromatographic Techniques

Molecular weight determination, Principles, Instrumentation (basic components) and applications of gas chromatography, High Performance Liquid Chromatography (HPLC), and Size Exclusion Chromatography.

Recommended Books:

1. Campbell, D., Pethrick, R. A., & White, J. R. (2017). *Polymer characterization: physical techniques*. CRC press.
2. Barth, H. G., & Mays, J. W. (Eds.). (1991). *Modern methods of polymer characterization* (Vol. 115). John Wiley & Sons.
3. Crompton, T. R. (2013). *Thermal methods of polymer analysis*. Smithers RAPRA.
4. Stuart, B. H. (2008). *Polymer analysis*. John Wiley & Sons.
5. Yang, R. (2018). *Analytical methods for polymer characterization*. CRC Press.
6. Briggs, D. (1998). *Surface analysis of polymers by XPS and static SIMS*. Cambridge University Press.

Course Structure of Ph. D. Program in Applied Physics
(Approved by AC.40/2021/2/3.5, AC.43/2022/2/3.1)

A student must complete minimum 16 credits including 'Doctoral Research Methodology' in the Department of Computer Science & Engineering (CS 704) and 'Ethics in Research' as the compulsory courses. The rest of the credits can be earned by completing at least one course from the Department of Applied Sciences, and courses from Department of Physics, or Open Elective, or MOOCs.

Course Code	Course Name	L-T-P	CH	Credit	Remarks
CS 704	Doctoral Research Methodology	4-0-0	4	4	Offered by the Department of Computer Science & Engineering
RP 799	Research and Publication Ethics	2-0-0	2	2	Offered by the School of Engineering
XXXX	Open Elective/ MOOC	x-x-x	x	3/4	Online platforms or courses offered by other departments
AP 701	Astrophysical Gas Dynamics and Accretion Process	3-1-0	4	4	Offered by the Department of Applied Sciences
AP 702	Optical Properties of Solids	3-1-0	4	4	Offered by the Department of Applied Sciences
AP 703	Introduction to Computational Methods and Applications	3-0-1	5	4	Offered by the Department of Applied Sciences (Approved by AC.44/2023/1/2.1)
PH 716	Surface Science	2-2-0	4	4	Offered by the Department of Physics
PH 717	Low Dimensional Structures	2-2-0	4	4	Offered by the Department of Physics
PH 723	Computer Basics and Simulation	2-1-1	5	4	Offered by the Department of Physics

PH 725	Introduction to the Interstellar Medium	2-2-0	4	4	Offered by the Department of Physics
PH 729	Statistical Methods and Data Analysis Techniques	2-1-1	5	4	Offered by the Department of Physics

AP 701: Astrophysical Gas Dynamics and Accretion Process **L-T-P-Cr-CH: 3-1-0-4-4**

Course Outcomes:

CO1. Recollect the basic equations of fluid mechanics and magnetohydrodynamics.
CO2. Recall the basic concepts of general relativity.
CO3. Identify the observed signatures of accretion discs in binary stars.
CO4. Recall the physics of accretion and accretion disc outbursts.
CO5. Analyze the X-ray emission of accreting compact bodies.
CO6. Determine the physics of astrophysical jets, gamma-ray bursts and active galactic nuclei.

Course Contents:

Unit 1: Basic Concepts of Gas Dynamics and Plasma Astrophysics
The equations of gas dynamics, steady adiabatic flows, isothermal flows, sound waves, plasma concepts, basic equations of MHD, Alfvén's theorem of flux freezing, shock waves in plasmas, basic concept of turbulence.

Unit 2: Basics of General Relativity
Basic concepts, Lorentz transformation, Minkowski space, general relativity: the equivalence principle and curvature of spacetime, tests of general relativity.

Unit 3: Accretion in Binary Systems
Interacting binary systems, Roche lobe overflow, Roche geometry and binary evolution, disc formation, viscous torques, the magnitude of viscosity, need of a turbulent viscosity.

Unit 4: Steady-State Accretion Discs
Eddington luminosity and accretion rate, spherically-symmetric accretion, radial disc structure, steady thin discs, the local structure of thin discs, spectrum of the disc, the structure of steady thermal dominated disc: α-disc, observational evidence for geometrically-thin optically-thick accretion discs.

Unit 5: Accretion Flows
Hot, non-thermal flow: advection-dominated accretion flow (ADAF)/ two-component accretion flow (TCAF)/ radiatively inefficient accretion flow (RIAF), spectrum of an ADAF, slim and thick discs.

Unit 6: X-ray emission and X-ray variability
Basic aspects of radiative transfer and radiative processes, thermal and non-thermal X-ray emission, classifications of X-ray binaries and their basic properties, X-ray bursters, periodic intensity dips, stochastic variability in X-ray emission: broadband noise and quasi-periodic oscillations.

Unit 7: Relativistic Outflows and Gamma-ray bursts

Relativistic jets, superluminal motion, gamma-ray bursts: discovery and breakthroughs, observed properties, constraints on GRB models, the fireball model, the central engine, other signatures and applications.

Unit 8: Accretion discs in AGN

Introduction to Active Galactic Nuclei (AGN), range of activity in 'Active' galaxies, the unified model of AGN: the central engine, evidence for the existence of supermassive black holes, jets, overall spectrum ofan AGN: accretion discs in AGN.

Text Books:

1. Accretion Power in Astrophysics. J. Frank, A. King and D. Raine, Cambridge University Press,3rd Edition, 2002.
2. High Energy Astrophysics: An Introduction. T. J.-L. Courvoisier, Springer, 2013th edition, 2012.
3. Extreme Environment Astrophysics. U. Kolb, Cambridge University Press, First published 2010.

References:

1. Exploring the X-ray Universe. F. D. Seward and P. A. Charles, Cambridge University Press, 2ndEdition, 2010.
2. The High Energy Universe. P. Mészáros, Cambridge University Press, Illustrated Edition, 2010.
3. High Energy Astrophysics. M. S. Longair, Cambridge University Press, 3rd Edition, 2011.
4. Black Holes, White Dwarfs, and Neutron Stars: The Physics of Compact Objects. S. L. Shapiroand S. A. Teukolsky, Wiley-VCH, 1st Edition, 1983.
5. The Physical Universe: An Introduction to Astronomy. F. Shu, University Science Books, 1981stEdition, 1981.
6. Radiative Processes in Astrophysics. G. B. Rybicki and A. P. Lightman, Wiley-VCH, 1st Edition,1985.
7. Astrophysics For Physicists. A. R. Choudhuri, Cambridge University Press, Print publicationyear:2010.

AP 702: Optical Properties of Solids **L-T-P-Cr-CH: 3-1-0-4-4**

Course Outcomes:

CO1. Identify the most important concepts and principles underlying various observed optical propertiesof solids in general.

CO2. Interpret the results of common optical experiments performed in his/her research from the understanding of the working principle of various experimental techniques.

CO3. Solve research problem by analyzing optical spectra obtained from experimental set up likephotoluminescence, Raman spectroscopy, spectroscopic ellipsometry.

CO4. Design new experiments based on the fundamental understanding of the optical properties of solidsand relevant experimental techniques.

CO5. apply the understanding of optical properties of novel low-dimensional solids like MoS2, graphenefor their utilization in the design of optoelectronic devices.

Course Contents:

Unit 1: Introduction

Maxwell's equations, refractive index and dielectric constant, Quantum mechanics and bandstructure

Unit 2: Classical and Quantum Mechanical Description

Drude and Lorentz models. Kramers-Kronig relationship, dispersion, birefringes

Unit 3: Interband Transitions and Semiconductor Optics

Transition rate, Direct gap and indirect gap semiconductors, van Hove singularities, diamond/zincblend valence band, spin-orbit coupling, Landau levels, Franz-Keldysh effect, semiconductor optoelectronic devices.

Unit 4: Excitons

Frenkel vs. Wannier excitons, optical selection rules, effect of Coulomb interaction on interband absorption, Optical spectra of excitons

Unit 5: Luminescence

Light emission in solids, interband luminescence, Photoluminescence, Electroluminescence

Unit 6: Semiconductor Quantum Wells

Quantum confined structures, excitons in quantum wells, quantum dots

Unit 7: Phonons

Infrared active phonons, infrared reflectivity and absorption in polar solids, polaritons, polarons, inelastic light scattering

Unit 8: Metals: Free Carrier Absorption and Plasmons
Free carrier absorption, plasma reflectivity, plasmons, screening, random phase approximation, lindhard dielectric response, anomalous skin effect, surface plasmons, plasmons in metallic particles

Unit 9: Impurity Centers
Semiconductors: electronic spectrum of shallow donors, multiple valleys, practical applications

Unit 10: Optical Properties of Nanoparticles
Mie Theory, Intrinsic and Extrinsic effect on optical properties of nanoparticles.

Unit 11: Experimental Techniques
Spectroscopic ellipsometry, Raman spectroscopy, photoluminescence, scanning near-field optical microscopy

Unit 12: Optical Properties of Two-Dimensional Materials
Optical properties of graphene, transition metal dichalcogenides (TMDC), valley selective absorption in TMDCs

Text Books:

1. Optical Properties of Solids. M. Fox, Oxford University Press, 2001.
2. Optical Processes of Solids. Y. Toyozawa, Cambridge University Press, 2003.

References:

1. Fundamentals of Semiconductors. P. Y. Yu and M. Cardona, Springer, 4th Edition, 2010.
2. Electrodynamics of Solids: Optical Properties of Electrons in Matter. M. Dressel and G. Gruner,Cambridge University Press, 2002.
3. Optical Properties of Solids. F. Wooten, Academic Press, 1972.

AP 703: Introduction to Computational Methods and Applications L-T-P-CR-CH: 3-0-1-4-5

Prerequisites: Nil

Course Objectives

CO1. To provide an introduction to computational methods in solving problems in physics and mathematics.

CO2. To familiarize with the main computational tools which permit to model and analyze the dynamic behavior of a wide range of physical problems.

CO3. To demonstrate the modeling/programming techniques for applying numerical methods to real physical problems.

Course outcomes

On successful completion of the course, the student will:

LO1. consider the numerical and algorithmic principles covered in the course and relate them to other numerical/computational methods from other courses in the curriculum.

LO2. recognize contemporary programming techniques and characterize the scope and constraints of computational methods.

LO3. be able to create a strategy for solving a given problem using one or more computational techniques, turn that strategy into concrete code, run the code, and then evaluate the output.

LO4. be able to use and develop concepts and methods for modeling the dynamic behavior of complex systems and the accompanying data analysis approaches.

LO5. read the current literature and appreciate the various approaches to numerical analysis for scientific and engineering applications.

Course content

Unit 1: Introduction, Numbers and their accuracy, Floating point arithmetic, errors in numbers, Computational methods for error estimation, General error formulae-approximation of a function, series approximations and error propagation in computation.

Unit 2: Fitting experimental data with parametrized models, the method of maximum likelihood, least square method, linear chi-square solution, non-linear least square fit, convergence criteria, least square fit with constraints, fit quality tests.

Unit 3: Revision of some basic concepts on polynomial equations, Bisection method, iterative method, Regula-falsi method, Newton-Raphson method, Secant method, Generalized Newton's method for multiple roots, solution of non-linear simultaneous equations and finding complex roots by Newton-Raphson method, solutions of systems of nonlinear equations, Numerical methods for computing approximate eigenvalues and eigenvectors.

Unit 4: Revision of basic properties of matrices and determinants, Matrix inversion and solution of transcendental and system of algebraic equations-Gauss elimination method, Jacobi's method and Gauss-Seidal method, Eigen values and eigen vectors.

Unit 5: Finite differences and difference operators, Newtons interpolation formulae, Gauss forward and backward formulae, Sterling, Bessel's and Evertte's formulae, Interpolation with unevenly spaced data points-Lagrange's interpolation, Hermite interpolation and Cubic spline interpolation.
Unit 6: Numerical differentiation, errors in numerical differentiation, Maximum and minimum values of a tabulated function, Numerical integration-Trapezoidal, Simpson's 1/3 rules, Boole's rule, Romberg integration-recursive formulae, Evaluation of double integrals by Trapezoidal and Simpson's rules, Gauss quadrature.
Unit 7: Taylor's series method, Picard's method, Euler's method, Modified Euler's method, Runge-Kutta methods of 2nd and 4th order, Adams-Moulton and Milne's methods, Solution of simultaneous and higher order equations, Initial value problem, Boundary value problem: Finite difference solutions to hyperbolic, parabolic and elliptic partial differential equations, application to physics problems, stability of single step and multistep methods, consistency and stability (by matrix method and Von Neumann method).

List of Fortran/Python/Java Computer Programs:

Program 1: Write a program to compute the real roots of a quadratic equation.

Program 2: Write a program to sort a given list of numbers in ascending or descending order.

Program 3: Write a program to compute the value of **exp**(x) for x = 0.5. Compare the result with exact solution obtained from the library function of Fortran/Python/Java.

Program 4: The velocity of a falling parachutist is given by

$$\boldsymbol{v = \frac{gm}{c}(1 - e^{-(c/m)t})}$$

where g = 9.8 m/s^2 . For a parachutist with a drag coefficient c = 15 kg/s, compute the mass m so that the velocity is v = 35 m/s at t = 8 s. Use the bisection method and false-position method to determine m to a level of $\boldsymbol{\varepsilon_s}$ = 0.1%.

Program 5: The state of an imperfect gas is given by van der Waals' equation

$$\boldsymbol{\left(p + \frac{\alpha}{v^2}\right)(v - \beta) = RT}$$

or

$$\boldsymbol{pv^3 - (\beta p + RT)v^2 + \alpha v - \alpha\beta = 0}$$

Solve the equation for v (molar volume) given the following:

p (pressure) = 1.1

T (temperature) = 250° K

R (gas constant) = 0.082

α = 3.6

β = 0.043

Use any suitable method.

Program 6: Use Gauss elimination to solve:

$$4x_1 + x_2 - x_3 = -2$$
$$5x_1 + x_2 + 2x_3 = 4$$
$$6x_1 + x_2 + x_3 = 6$$

Check your answers by substituting them into the original equations.

Program 7: The following system of equations is designed to determine concentrations (the *c*'s in g/m^3) in a series of coupled reactors as a function of the amount of mass input to each reactor (the right-hand sides in g/day),

$$15c_1 - 3c_2 - c_3 = 3300$$
$$-3c_1 + 18c_2 - 6c_3 = 1200$$
$$-4c_1 - c_2 + 12c_3 = 2400$$

(a) Determine the matrix inverse.

(b) Use the inverse to determine the solution.

(c) Determine how much the rate of mass input to reactor 3 must be increased to induce a 10 g/m^3 rise in the concentration of reactor 1.

(d) How much will the concentration in reactor 3 be reduced if the rate of mass input to reactors 1 and 2 is reduced by 700 and 350 g/day, respectively?

Program 8: Use Gauss-Jordan elimination to solve:

$$2x_1 + x_2 - x_3 = 1$$
$$5x_1 + 2x_2 + 2x_3 = -4$$
$$3x_1 + x_2 + x_3 = 5$$

Do not employ pivoting. Check your answers by substituting them into the original equations.

Program 9: Write a program to find the inverse of a given matrix **A** by the partition method and show that $\mathbf{AA^{-1} = I}$.

Program 10: Write a program to solve a given set of linear equations using Jacobi iteration method.

Program 11: Write a program to solve a given system of equations by Gauss-Seidel iteration method using $x_0 = 0$, $y_0 = 0$ and $z_0 = 0$.

Program 12: Write a program to find the curve of best fit of the type $y = ax + bx^{-0.5}$ to given data by the method of least square and find the least square error.

Program 13: Write a program to use the linear interpolation method and determine the value of the square root of a given integer from given data.

Program 14: Write a program for computing the interpolated value at a specified point, given a set of data points, using the Lagrange interpolation polynomial.

Program 15: Write a program to estimate the natural logarithm of a given integer following linear interpolation method using given data.

Program 16: Write a program to fit a second order polynomial (Quadratic Interpolation) to given data points. Use the polynomial to evaluate natural logarithm of a given integer.

Program 17: Write a program to use third order polynomial and estimate natural logarithm of a given integer for given data points.

Program 18: Write a program to use a Lagrange interpolating polynomial of the first and second order to evaluate natural logarithm of a given integer on the basis of given data. Compare the values of natural logarithm of the given integer obtained from four different approaches.

Program 19: The viscous resistance of an object moving through a fluid with velocity v is given by

$$\boldsymbol{R = -v^{3/2}}$$

The velocity is decreased with time t. The time taken for the velocity to decrease from v_0 to v_1 is given by

$$\boldsymbol{T = \int_{v_0}^{v_1} \frac{m}{R} dv \text{ seconds} = -\int_{v_0}^{v_1} \frac{m}{v^{3/2}} dv \text{ seconds}}$$

where m is the mass of the object. Estimate using both Trapezoidal rule and Simpson's 1/3 rule, the time T required for an object with m = 30 kg to reach a velocity of 10 m/sec from an initial velocity of 20 m/sec.

Program 20: A spherical tank has a circular orifice in its bottom through which the liquid flows out. The flow rate through the hole can be estimated as

$$\boldsymbol{Q_{out} = CA\sqrt{2gH}}$$

where $\boldsymbol{Q_{out}}$= outflow (m^3/s), C = an empirically-derived coefficient, A = the area of the orifice (m^2), g = the gravitational constant (= 9.81 m/s^2), and H = the depth of liquid in the tank. Use the fourth-order RK method to determine how long it will take for the water to flow out of a 3-m diameter tank with an initial height of 2.75 m. Note that the orifice has a diameter of 3 cm and C = 0.55.

Program 21: Solve for the steady-state temperatures in a rectangular plate 8 cm × 10 cm, if one 10 cm side is held at 50°C, and the other 10 cm side is held at 30°C and the other two sides are held at 10°C. Assume square grids of size 2 cm × 2 cm.

Textbooks:

- Balagurusamy, E., *Numerical Methods*, McGraw Hill Education (India) Private Limited, 2018
- Chapra, S. C. and Canale, R. P., *Numerical Methods for Engineers*, Tata McGraw Hill Education Private Limited, 2007

References:

- Sastry, S. S., *Introductory Methods of Numerical Analysis*, PHI Learning Private Limited, 2012
- Rajamaran, V., *Computer Oriented Numerical Methods*, Prentice-Hall of India Private Limited, 2006

- Press, W. H., Flannery, B. P., Teukolsky, S. A. and Vetterling, W. T., *Numerical Recipes in FORTRAN 77: The Art of Scientific Computing*, Cambridge University Press, 1992
- Das, P. S. and Vijayakumari, C., *Numerical Analysis*, Pearson, 2014
- Kincaid, D. and Cheney, W., *Numerical Analysis: Mathematics of Scientific Computing*, 3rd Edn., AMS, 2002
- Atkinson, K. E., *Introduction to Numerical Analysis*, 2nd Edn., John Wiley, 1989
- Conte, S. D. and Boor, Carl de, *Elementary Numerical Analysis - An Algorithmic Approach*, 3rd Edn., McGraw Hill, 1980