

List of external participants confirmed so for participation in "Hands on Training cum Workshop on Soft Computing Skill for Scientists and Engineers" 17-19 March 2017.

S. No./Ref.	Name of the Participant	Faculty/ Research Scholar/M.Tech	Name of the Institute
SCSSSE-1731	Majhrul Israr	M.Tech	MMMUT,GKP
SCSSSE-1732	Mithilesh Kumar Kanaujia	Faculty	GITI, GKP
SCSSSE-1733	V P Yadav	Faculty	GITI, GKP
SCSSSE-1734	B B Nath Anchal	Research Scholar	IIT, BHU
SCSSSE-1735	K K Gautam	Faculty	REC, Bijnaur
SCSSSE-1736	Ms. Vandana Rao	Research Scholar	DDU, GKP
SCSSSE-1737	Parvej Ansari	Faculty	KIPM, GKP
SCSSSE-1738	Rahul Patel	Faculty	KIPM, GKP
SCSSSE-1739	Hanuman Maurya	Faculty	REC, Bijnaur
SCSSSE-1740	Ajay K Maurya	Guest Faculty	MMMUT,GKP
SCSSSE-1741	Shivani Gupta	M.Sc	DDU, GKP
SCSSSE-1742	Dr. Naresh K Chaudhary	Faculty	Dr.R ML AU, Faizabad
SCSSSE-1743	Avinash Kumar Pandey	Research Scholar	DDU, GKP
SCSSSE-1744	Abhishek Kumar Mishra	Research Scholar	DDU, GKP
SCSSSE-1745	Amit Kumar Vishwakarma	Research Scholar	DDU, GKP
SCSSSE-1746	Juhi Gupta	M. Sc.	DDU, GKP
SCSSSE-1747			
SCSSSE-1748			
SCSSSE-1749			
SCSSSE-1750			

Note: The participants are requested to be present at registration desk at 9:00 am sharp on 17th March 2017. On spot registration is possible depending on availability of seats.

Cordinator

Program Schedule

17th March 2017 (Friday) – DAY I

9:30 Inauguration by Honourable Vice Chancellor

10:00 High Tea

10:15 Introduction to Mathematica

- Basics of Mathematica
- Notebook Interface
- Wolfram Alpha
- Creating Dynamic models
- Publishing paper

10:45 Programming with Wolfram Language

- What is Functional Programming
- Rules of Writing Codes
- Direct and Delayed Assignments

11:15 Symbolic and Numeric Computation

- Numbers and Precision
- Matrices and Linear Algebra
- Equation Solving
- Calculus
- DEs and PDEs Solving

12:15 Visualization using Mathematica

- Function Visualization
- Data Visualization
- Dynamic Visualization

13:15 Lunch

14:00 Hands on Session I

- Creating Dynamic Models

15:00 Tea Break

15:15 Hands On Session II

- 2nd order PDE & how to solve

16:15 Hands On Session II

- Parallel computing using Mathematica
- Signal Processing
- Image Processing

17:15 Wolfram Links

17:30 Departure

18th March 2017 (Saturday) – DAY II

09:30 Introduction to Gaussian

09:45 Geometry Optimization

- Potential Energy Surface.
- Geometry Optimization I (Minimization)
- Geometry Optimization II (Transition Structures)

10:30 Vibrational Spectroscopy, Thermochemistry And Model Chemistry

11:00 High Tea

11:15 Methods in Gaussian

- Semi- Empirical
- Molecular Mechanics Methods
- ab-initio Methods and Solvation Methods and Basis Sets

12:15 Running Gaussian Jobs

- Gaussian Job Files and Analysing output

13:15 Lunch

14:00 Laboratory I

- Welcome to GaussView
- Building Molecules

14:30 Laboratory II

- Running Electronic Structure Calculation I
- Visualizing Spectra
- From Gas to Solution Phase

15:15 Tea Break

15:30 Laboratory III

- Investigating Chemical Reactions I
- Analyzing Electronic Structure Results I
- Visualizing Orbitals

16:30 Laboratory IV

- Investigating Chemical reaction II
- Visualizing Spectra II
- Analyzing Electronic Structure Results II
- Visualizing Spectra III

17:00 Departure

19th March 2017 (Sunday) – DAY - III

9:30 Introduction to CONFLEX: High Performance Conformational Analysis software

10:30 Vote of Thanks and Certificate distribution

11:30 Tea and Departure