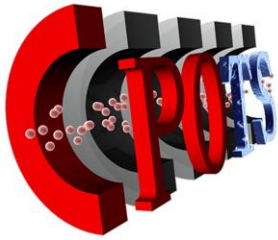


CHARGED PARTICLE OPTICS – THEORY AND SIMULATION (CPOTS)



Erasmus Intensive Programme

Physics Department University of Crete

August 28 – September 11, 2011

Heraklion, Crete, Greece

Participating Institutions and Instructors

1. University of Crete (UoC)

- **Prof. Theo Zouros*** (Project coordinator)
- Prof. Fanis Kitsopoulos

2. Afyon Kocatepe University (AKU)

- **Prof. Mevlut Dogan** (contact)
- Prof. Melike Ulu*
- Dr. Omer Sise*
- Zehra Nur Erengil*

3. Selçuk University (SU)

- **Prof. Hamdi Sukur Kilic** (contact)

4. Universidad Computense Madrid (UCM)

- **Prof. Genoveva Martinez - Lopez** (contact)

5. University of Ioannina (Uoi)

- **Prof. Manolis Benis*** (contact)

6. Technische Universität Wien (TUW)

- **Prof. Fritz Aumayr** (contact)
- Dr. Gregor Kowarik*

Brookhaven National Laboratories

- **Prof. Nick Tsoupas*** (invited)

*SIMION user

General IP rules and participant information

- **Attendance sheet**

An attendance sheet will be maintained for all lectures and labs for all participants (teachers and students).

- **Teachers**

1. Minimum suggested stay at an Erasmus IP including travel both ways: **5 days** (as certified by the attendance sheet).
2. Minimum number of suggested lecturing hours at an Erasmus IP: **5 hours** (as certified by the attendance sheet).
3. A minimum of **three** laboratory instructors will be available at every afternoon laboratory session.
4. The instructor in charge of each unit will be responsible for:
 - i) The proper execution of the lectures as described in the work program.
 - ii) The accreditation quiz at the end of the unit. Contributions to the quiz will be prepared by all lecturers of the unit.
 - iii) The material (simulations, etc.) of the corresponding afternoon laboratory.

- **Students**

1. A CPOTS2011 Certificate of Attendance will be given to students who are present **at all lectures/labs within the 10 day work programme of the IP** (as certified by the attendance sheet).
2. 6 ECTS will be given to all students with the CPOTS2011 Certificate of Attendance that have **passed the course**. A final grade of 5.0 (out of 10) or greater will be required for passing.
3. The course grade will be determined by a weighted average of grades obtained from the exams, class participation and a possible project (group or individual). The final course grade algorithm will be defined as the lectures and lab simulations are closer to completion.
4. The course will have 5 quizzes one for each of the 5 units of the IP. Each quiz will be given at the end of each unit as indicated in the work program. The final exam grade will be determined from the average of the 5 quizzes.

1. Transport of Charged Particle Beams

(Genoveva Martinez Lopez – GML, Nikos Tsoupas – NT)

1.1 Charged particle motion in Electromagnetic Fields *(GML)*

Lorentz force equation. Electron trajectories in static electric and magnetic fields. Relativistic case. Final remarks.

1.2 Numerical methods for solving Laplace equation *(GML)*

Finite Difference Method (FDM): Mathematical preliminaries. Iterative solution and relaxation techniques. Examples.

Boundary Element Method (BEM): Integral formulation for a set of conductors. Boundary conditions and discretisation. Solving the system of equations: approximate charge distribution. Example.

Finite Element method (FEM): Mesh discretisation. Element governing equations. Assembling of all elements and solving the resulting equations. Example.

1.3 Numerical methods for the calculation of charged particle trajectories *(GML)*

Numerical integration of Newton's equations including velocity dependent forces: Euler-Richardson method. Runge-Kutta methods. Multi-step methods. SIMION's numerical integration method.

1.4 Gaussian Optics and Transfer Matrices *(GML+NT)*

1.4a Gaussian approximation. Ideal imaging properties: fundamental rays and cardinal points (GML).

1.4b Introducing the Lorentz Force. Brief introduction to Maxwell's Equations. Pictures of some magnets which are used to guide and focus charged particles. Solution of the equation of motion of a single particle moving in a uniform magnetic field (use of Cartesian coordinate system). Definition of the reference orbit and the reference (central) particle. Introduction to the curvilinear coordinate system (a simplified Frenet-Serret coordinate system). Express the differential equation of motion of a particle in a magnetic field (Lorentz force) in the curvilinear coordinate system. Examples of solving the equations of motions in the curvilinear system for a particle moving: a) Along the central trajectory, b) In Uniform magnetic field, c) In a quadrupole field (Hill's equation). Example of using the transfer matrix formalism: focusing-defocusing set of quadrupoles in the thin lens approximation. Stability criterion of a particle transported by a FODO lattice. (NT)

1.5 First order Beam Transport (NT)

Properties of the R matrix. Linear transformation of an ellipse. Linear Transport of a beam. Linear Transport of a beam having a Gaussian distribution.

1.6 Phase Space, Beam Emittance and Liouville's theorem (NT)

Define phase space. Conservation of phase space. Liouville's theorem. Define beam emittance Geometrical and normalized beam emittance. One method to measure the beam emittance.


1.7 Aberrations in CPO (GML)

Geometrical aberrations of electron optics imaging systems: aberration figures. Chromatic and asymmetric aberrations. General scheme for the calculation of aberrations.

1.8 ECTS accreditation quiz on Unit 1 (GML+NT)

Exam on Unit 1 for those participants who have applied for the 6 ECTS units.

Bibliography

- [1] *Application of the integral equation method to the analysis of electrostatic potentials and electron trajectories*, Genoveva Martinez and M. Sancho, *Advances in Electronics and Electron Physics* **81** (1991) 1-41  (24MB)
- [2] Mikhail I. Yavor, *Optics of Charged Particle Analyzers*, *Advances in Imaging and Electron Physics*, (Academic Press, Amsterdam 2009), vol. 157, pp. 373.
- [3] H. Wollnik, *Optics of Charged Particles*, (Academic Press, London, 1987) pp. 291.
- [4] R.F. Harrington, *Field Computation by Moment Methods*, (New York: Mcmillan, 1968).
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- [6] COMSOL Multiphysics, <http://www.comsol.com>
- [7] D. Griffiths, *Introduction to Electrodynamics*, (New Jersey: Prentice Hall, 1999).
- [8] W.H. Press et al., *Numerical Recipes*, (Cambridge University Press, 1992) pp. 701.
- [9] S. Y. Lee, *Accelerator Physics*, (World Scientific, 1999).
- [10] A. Septier editor, *Focusing of charged particles*, (Academic Press, 1967).
- [11] Karl L. Brown, Roger V. Servranckx, SLAC-PUB-3381 July 1984 (A).
- [12] H. Wiedermann, *Particle Accelerator Physics Basic Principles and Beam Dynamics*, (Springer-Verlag, 1993).

L1. Simulation Laboratory

(Theo Zouros – TZ, Manolis Benis – MB, Omer Sise – OS, Melike Ulu – MU, Gregor Kowarik – GK)

L1.1 Quick tour of SIMION 8 (TZ)

Main concepts, SIMION GUI, Workbench concept (IOB file), REC, FLY, and ION files, Coordinate system: azimuth, elevation, Units: gu, mm, in. Workbench and PA coordinates. Contours, Potential energy maps. Flying Ions: Definition of ions, Data recording. Solving Laplace's equation: Refining, Fast adjusting. Trajectory calculation: Runge-Kutta, Variable time steps, PRG programs. Ways to create geometries: GEM files. Limitations of SIMION. Resources: Simion.com – FAQ, tutorials, papers, manual + course notes

L1.2 SIMION: Flying Ions and Recording results (OS)

Ion Definitions, Defining Ions in Groups (.FLY, .FLY2), Defining Ions Individually (.ION) Defining Ions Outside of SIMION (.ION), Data Recording (.REC), Data Recording to a File, What, When, How, and Where to record, Using the Data Monitoring Screen, Recording Trajectories (.TRJ)

L1.3 SIMION: Creating and Refining 2D and 3D Potential Arrays, Geometry files and Ion Optical Bench (MB)

.PA, .PA#, .PAO files, .GEM files

Discuss Modify with 3D Arrays, 2D to 3D and 3D to 2D Conversions, 3D Layers and Marking in Modify, Find Options Replace, Edge, Move, Copy, and etc., Discuss the Double and Halve Functions

Creating Arrays with Geometry Files, Pros and Cons of Geometry Files, Nested Structure Used in Geometry Files, Locate Command

L1.4 SIMION: User Programming Concepts (GK)

Time-of-flight concepts, Instances, Recording fly data with User Programs .PRG files, .lua files

L1.5 SIMION: Lua programming language (GK)

Basic commands and usage

L1.6 SIMION: Examples (OS, GK, MU)

Bibliography

[1] [SIMION info documentation](#)

[2] [SIMION 8 manual](#)

[3] SIMION 8 update Overview - Course Notes



[4] [Lua programming Language](#)

Physics Dept. Univ. Of Crete Heraklion

Program of Lectures and Labs

Unit 1: Transport of Charged Particle Beams

| Time | Section | Lecturer |
|----------------------|----------------------------------------------------------------------------|-------------------------------------------|
| Monday Aug 29 | | |
| 9:00-10:00 | 1.1 Charged particle motion in Electromagnetic Fields | Genoveva Martinez-Lopez |
| 10:00-11:00 | 1.2 Numerical methods for solving Laplace equation | Genoveva Martinez-Lopez |
| 11:00-11:30 | Coffee Break | |
| 11:30-12:30 | 1.3 Numerical methods for the calculation of charged particle trajectories | Genoveva Martinez-Lopez |
| 12:30-13:30 | 1.4 Gaussian Optics and Transfer Matrices | Genoveva Martinez-Lopez, Nikos Tsoupas |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L1.1 Quick Tour of SIMION 8.0 | Theo Zouros (O Sise, M Benis) |
| 15:30-16:30 | L1.2 SIMION: Flying Ions and Recording results | Omer Sise (T Zouros, M Benis) |
| 16:30-17:30 | L1.3 SIMION: Geometry files and Ion Optical Bench | Manolis Benis (T Zouros, O Sise) |

Tuesday Aug 30

| | | |
|-------------|---------------------------------------------------------|---------------------------------------------|
| 9:00-10:00 | 1.5 First order Beam Transport | Nikos Tsoupas |
| 10:00-11:00 | 1.6 Phase Space, Beam Emittance and Liouville's theorem | Nikos Tsoupas |
| 11:00-11:30 | Coffee break | |
| 11:30-12:30 | 1.7 Aberrations in CPO | Genoveva Martinez-Lopez |
| 12:30-13:30 | 1.8 ECTS ACCREDITATION exam on Unit 1 | G. Martinez-Lopez, N. Tsoupas, H S Kilic |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L1.4 SIMION: Programming Concepts | G Kowarik (O Sise, M Ulu) |
| 15:30-16:30 | L1.5 SIMION: Lua Programming Language | G Kowarik (O Sise, M Ulu) |
| 16:30-17:30 | L1.6 SIMION: Examples | G Kowarik, O Sise, M Ulu |

Each 1 hour lecture should allow for 10 minutes discussion/questions.

2 Focusing Systems - Lenses

(Omer Sise - OS, Melike Ulu - MU, Mevlut Dogan – MD, Nikos Tsoupas – NT)

2.1 Introductory Guide to Electrostatic Lenses (MU)

Electrostatic lenses are fairly simple static field systems, often with 2D cylindrical symmetry. They are widely used in conjunction with other electron/ion spectrometer components and are easy to simulate. Understanding their simulation forms the basis for simulating other systems. Why we need electrostatic lenses? Basic tools of the trade. Optical Analogy. Snell's Law. Significant differences. Lens Parameters. Focal and Principal Planes. Electron Optical Properties. Helmholtz-Lagrange Law. Thin Lenses. Matrix Method

2.2 Focal and Zoom Lens Properties (OS)

Lens types: Aperture or Cylinder. Two-element lens. P-Q diagrams. Three-element lens. Zoom lenses. Paraxial Approximation & Aberrations. Spherical Aberration. Figures of merit, g and g_0 . Chromatic Aberration. Aberration Pattern

2.3 Computation of Parameters of Some Electrostatic Lenses (OS)

Three-Element Lenses. Four-Element Lenses. Five-Element Lenses

2.4 Applications of Electrostatic Lenses (MD)

Electron guns. Entrance optics of energy analyzers. Other examples

2.5 Magnetic Lenses (NT)

Brief Introduction on magnetic lenses. Taylor series expansion of the magnetic scalar potential ϕ , in the curvilinear coordinate system. Express the magnetic field components in the curvilinear coordinate system, correct to third order in coordinates. The Quadrupole as a magnetic lens. Applications to beam transport and beam focusing. The concept of aberrations in beam optics What aberrations are. A non-mathematical introduction.

2.6 Magnetic Sector Field Lenses (NT)

The deflecting magnet and some of its properties. Horizontal focusing by a sector magnet. Hard edge horizontal focusing by a dipole magnet. Fringe field vertical focusing by a dipole magnet. Aberration coefficients, first second and third order aberration coefficients and beam focusing. Edge focusing and reduction of higher order aberrations

2.7 Other software packages (OS+NT)

LENSYS and How to design a magnet with OPERA – a simple example

2.8 ECTS accreditation exam on Unit 2 (OS +MU+MD+NT)

Physics Dept. Univ. Of Crete Heraklion

Exam on Unit 2 for those participants who have applied for the 6 ECTS units.

Bibliography

- [1] Mikhail I. Yavor, [Optics of Charged Particle Analyzers](#), Advances in Imaging and Electron Physics, (Academic Press, Amsterdam 2009), vol. 157, pp. 373.
- [2] D. W. O. Heddle, *Electrostatic Lens Systems*, 2nd edition (Institute of Physics Publishing, Bristol, 2000) pp. 128.

L2. Simulation Laboratory

(Omer Sise - OS, Melike Ulu - MU, Zehra Nur Erengil - ZNE)

L2.1 SIMION modules for lenses (*OS, MU, ZNE*)

L2.2 SIMION modules for lenses (*OS, MU, ZNE*)

L2.3 SIMION modules for lenses (*OS, MU, ZNE*)

L2.4 SIMION modules for electron guns (*OS, MU, ZNE*)

L2.5 SIMION entrance optics of energy analyzer (*OS, MU, ZNE*)

L2.6 SIMION modules on ... (*OS, MU, ZNE*)

Bibliography

[1] [SIMION 8 manual](#)

[2] SIMION 8 update Overview - Course Notes



Program of Lectures and Labs

Unit 2: Focusing systems - Lenses

| Time | Section | Lecturer |
|-------------------------|------------------------------------------------------------|------------------------------------|
| Wednesday Aug 31 | | |
| 9:00-10:00 | 2.1 Introductory Guide to Electrostatic Lenses | Melike Ulu |
| 10:00-11:00 | 2.2 Focal and Zoom Lens Properties | Omer Sise |
| 11:00-11:30 | Coffee Break | |
| 11:30-12:30 | 2.3 Computation of Parameters of Some Electrostatic Lenses | Omer Sise |
| 12:30-13:30 | 2.4 Applications of Electrostatic Lenses | Mevlut Dogan |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L2.1 SIMION modules for lenses | O Sise, M Ulu, ZN Erengil, M Dogan |
| 15:30-16:30 | L2.2 SIMION modules for lenses | O Sise, M Ulu, ZN Erengil, M Dogan |
| 16:30-17:30 | L2.3 SIMION modules for lenses | O Sise, M Ulu, ZN Erengil, M Dogan |

Thursday Sept 1

| | | |
|-------------|------------------------------------------------|-----------------------------------------------------------------|
| 9:00-10:00 | 2.5 Magnetic Lenses | Nikos Tsoupas |
| 10:00-11:00 | 2.6 Magnetic Sector Field Lenses | Nikos Tsoupas |
| 11:00-11:30 | Coffee break | |
| 11:30-12:30 | 2.7 Other software packages: LENSYS | Omer Sise, Nikos Tsoupas |
| 12:30-13:30 | 2.8 ECTS ACCREDITATION exam on Unit 2 | O Sise, M Ulu, G Martinez-Lopez, M Dogan, N. Tsoupas, H S Kilic |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L2.4 SIMION modules for electron guns | O Sise, M Ulu, ZN Erengil, M Dogan |
| 15:30-16:30 | L2.5 SIMION entrance optics of energy analyzer | O Sise, M Ulu, ZN Erengil, M Dogan |
| 16:30-17:30 | L2.6 SIMION: Examples | O Sise, M Ulu, ZN Erengil, M Dogan |

Each 1 hour lecture should allow for 10 minutes discussion/questions.

3. Energy and Momentum Analyzers

(Theo Zouros-TZ, Nikos Tsoupas-NT)

3.1 Charged Particle Analyzers (TZ)

Typical uses of analyzers, spectrometers and spectrographs. Basic concepts: dispersion, focusing, transmission, luminosity, Etendue, energy (momentum) resolution, angular resolution, central trajectory equation, chromatic and angular aberrations. Focusing: single focusing, double focusing, 1st order, 2nd order, solid angle, resolution, pre-retardation, dispersion, trace width, line profile, base width, FWHM. Figures of merit, fringing fields, Barber's rule, Helmholtz-Lagrange law, multiple stage spectrometers, μ -metal screening, Simulations. Electrostatic versus magnetostatic spectrometers

3.2 Energy Dispersion and Electrostatic Spectrometers (TZ)

Basic types of electrostatic spectrometers, Prisms and Mirrors, Parallel Plate Analyser, Fountain Analyser, Cylindrical Plate Analyser, Hemispherical Deflector Analyser, Cylindrical Mirror Analyser, Toroidal Analyser, Spherical Mirror Analyser.

3.3 Momentum Dispersion and Magnetic Spectrometers (NT)

Description of dispersive magnetic systems. Defining a magnetic spectrometer. Resolving power of a magnetic spectrometer. Applications of magnetic spectrometers. Design procedures of a magnetic spectrometer. Aberrations of a magnetic spectrometer

3.4 OPERA: Software design of electromagnetic devices (NT)

Brief description of the OPERA software code. Application to magnet design.

3.5 Case studies of basic Electrostatic Spectrometers (TZ)

Case study 1: Parallel plate Analyzer, basic trajectory equation, energy resolution, TOF, aberrations, 45 and 30 degree analyzers, pre-retardation, tandem. Simulations.

Case study 2: Hemispherical Deflector Analyser (HDA), basic trajectory equation, energy resolution, TOF, aberrations, fringing field correction, biased paracentric entry, injection lens, ultimate resolution of combined lens+HDA. Simulations.

3.6 Case studies of basic Magnetic Spectrometers (NT)

Examples of magnetic spectrometers. Design of split pole magnetic spectrometer. Magnetic shielding design.

3.7 TRANSPORT software code (NT)









A code for beam transport using magnetic elements. Brief description of the theoretical basis of the code. Various applications of the code. Examples.

3.8 ECTS accreditation exam on Unit 3 (TZ, NT)

Exam on Unit 3 for those participants who have applied for the 6 ECTS units.

Physics Dept. Univ. Of Crete Heraklion

Bibliography

- [1] Mikhail I. Yavor, [Optics of Charged Particle Analyzers](#), Advances in Imaging and Electron Physics, (Academic Press, Amsterdam 2009), vol. 157, pp. 373.
- [2] K. D. Sevier, *Low Energy Electron Spectrometry*, (Wiley, New York, 1972).
- [3] H. Wollnik, *Optics of Charged Particles*, (Academic Press, London, 1987) pp. 291.
- [4] E.H.A. Granneman and M.J. Van der Wiel, *Transport, dispersion and detection of electrons, ions and neutrals* in Handbook of Synchrotron Radiation, edited by E.E. Koch, (North Holland, Amsterdam, 1983) vol. 1A, Chapter 6, pp. 367-456. 
- [5] T.J.M. Zouros and E.P. Benis, *The hemispherical deflector analyser revisited. I. Motion in the ideal 1/r potential, generalized entry conditions, Kepler orbits and spectrometer basic equation*, [J. of Electron Spectroscopy and Rel. Phenom.](#) **125** (2002) 221-248  [Erratum](#) 
- [6] E.P. Benis and T.J.M. Zouros, *The hemispherical deflector analyser revisited. II. Electron-optical properties*, [J. of Electron Spectroscopy and Related Phenomena](#) **163** (2008) 28-39 
- [7] T.J.M. Zouros, Omer Sise, F.M. Spiegelhalter and David J. Manura, *Investigation of the accuracy of ion optics simulations using Kepler orbits in a spherical capacitor*, [International Journal of Mass Spectrometry](#) **261** (2007) 115-133 
- [8] B. Sulik and N. Stolterfoht, *Auger Electron Spectroscopy of Target Atoms* in Accelerator-based atomic physics techniques and applications, Eds. S M Shafroth and J C Austin (American Institute of Physics, Woodbury, NY, 1997), Ch. 12, pp. 377- 425. 
- [9] T J M Zouros and D H Lee, *Zero Degree Auger Electron Spectroscopy of Projectile Ions* in Accelerator-based atomic physics techniques and applications, Eds. S M Shafroth and J C Austin (American Institute of Physics, Woodbury, NY, 1997), Ch. 13, pp. 427 - 479. 
- [10] D Roy and D Tremblay, *Design of electron spectrometers*, [Rep. Prog. Phys.](#) **53** (1990) 1621-1674. 
- [11] Yves Ballu, *High Resolution Electron Spectroscopy* in Applied Charged Particle Optics, A. Septier (editor), Advances in Electronics and Electron Physics Supplement 13B, p. 257-371 (1980)

L3. Simulation Laboratory

(Theo Zouros – TZ, Nikos Tsoupas – NT, Gregor Kowarik - GK)

L3.1 SIMION modules on electrostatic spectrometers (*TZ, NT, GK*)

L3.2 SIMION modules on electrostatic spectrometers (*TZ, NT, GK*)

L3.3 SIMION modules on magnetostatic spectrometers (*TZ, NT, GK*)

L3.4 Simple beam line design using TRANSPORT (*TZ, NT, GK*)

L3.5 SIMION and OPERA modules on magnetostatic spectrometers (*TZ, NT, GK*)

L3.6 SIMION: Examples (*TZ, NT, GK*)

Bibliography

[1] [SIMION 8 manual](#)

[2] SIMION 8 update Overview - Course Notes



Program of Lectures and Labs

Unit 3: Energy and Momentum Analyzers

| Time | Section | Lecturer |
|----------------------|-------------------------------------------------------|------------------------------------|
| Friday Sept 2 | | |
| 9:00-10:00 | 3.1 Charged Particle Analyzers | Theo Zouros |
| 10:00-11:00 | 3.2 Energy Dispersion and Electrostatic Spectrometers | Theo Zouros |
| 11:00-11:30 | Coffee Break | |
| 11:30-12:30 | 3.3 Momentum Dispersion and Magnetic Spectrometers | Nikos Tsoupas |
| 12:30-13:30 | 3.4 OPERA: Software design of electromagnetic devices | Nikos Tsoupas |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L3.1 SIMION modules on electrostatic spectrometers | T. Zouros (N. Tsoupas, G. Kowarik) |
| 15:30-16:30 | L3.2 SIMION modules on electrostatic spectrometers | T. Zouros (N. Tsoupas, G. Kowarik) |
| 16:30-17:30 | L3.3 SIMION modules on magnetic spectrometers | N. Tsoupas (T. Zouros, G. Kowarik) |

Monday Sept 5

| | | |
|-------------|---------------------------------------------------------|----------------------------------------------------|
| 9:00-10:00 | 3.5 Case studies of basic Electrostatic Spectrometers | Theo Zouros |
| 10:00-11:00 | 3.6 Case studies of basic Magnetic Spectrometers | Nikos Tsoupas |
| 11:00-11:30 | Coffee break | |
| 11:30-12:30 | 3.7 TRANSPORT software code | Nikos Tsoupas |
| 12:30-13:30 | 3.8 ECTS ACCREDITATION exam on Unit 3 | T. Zouros, N. Tsoupas, G. Martinez-Lopez, M. Dogan |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L3.4 Simple beam line design using TRANSPORT | N. Tsoupas (T. Zouros, G Kowarik) |
| 15:30-16:30 | L3.5 SIMION and OPERA modules on magnetic spectrometers | N. Tsoupas (T. Zouros, G Kowarik) |
| 16:30-17:30 | L3.6 SIMION: Examples | T. Zouros, N. Tsoupas, G Kowarik |

Each 1 hour lecture should allow for 10 minutes discussion/questions.

4. Time of Flight Devices and Mass Analyzers

(Hamdi Sukur Kilic – HSK, Zehra Nur Erengil – ZNE, Manolis Benis -MB)

4.1 Mass Spectrometry (HSK)

Introduction, the concept of mass spectrometry, history, terminology. Ions. Peaks, resolution, resolving power.

4.2 Ion Sources (HSK)

Electron Ionization, Chemical Ionization, Electrospray Ionization, Photoionization, Multiphoton Ionization, Fast Atom Bombardment, Secondary Ion Mass Spectrometry, Laser Desorption/Ionization, Matrix-Assisted Laser Desorption/Ionization

4.3 Mass Analysers (HSK)

Types of Mass Analysers, Applications, Advantages and Disadvantages.

4.4 Time-of-Flight Mass Spectrometers (HSK)

Linear TOF Mass Spectrometer, Time of Flight Equation and Mass Resolution, Time, Space and Kinetic Energy Distribution, Time-Lag Focusing

4.5 Reflectron Time of Flight Mass Spectrometer (HSK)

History. Construction of Reflectron. Theoretical Information. Advantages and Disadvantages of the Reflectron. Construction of the Reflectron Simulation in SIMION. Kinds of Reflectrons. The Single-Stage Reflectron. The Dual-Stage Reflectron. Linear vs. Reflectron Instrument. The Mamyrin Reflectron. Applications: SIMION simulation of Reflectron

4.6 Important Applications of Mass Spectrometry (HSK)

- 4.6.1 **Femtosecond Laser Mass Spectrometry (FLMS):** Introduction of laser mass spectrometry, importance of short laser pulses in mass spectrometry, analysis of large molecules using FLMS techniques, comparison of some ns and fs laser mass spectra.
- 4.6.2 **Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS):** Introduction of the technique, importance and application areas of the LA-ICP-MS technique.


4.7 Special applications in TOF (MB, GK)

- 4.7.1 TOF in Magnetic bottle (MB).
- 4.7.2 Production of nanosecond pulsed beam using time-dependent electric field (GK).

4.8 ECTS accreditation exam on unit 4 (HSK, ZNE, MB)

Exam on Unit 4 for those participants who have applied for the 6 ECTS units.

Bibliography

- [1] Mikhail I. Yavor, [Optics of Charged Particle Analyzers](#), Advances in Imaging and Electron Physics, (Academic Press, Amsterdam 2009), vol. 157, pp. 373.
- [2] Benjamin Whitaker (Ed.), [Imaging in Molecular Dynamics - Technology and Applications \(A user's guide\)](#) (Cambridge University Press, Cambridge, 2003) pp. 247.
- [3] P. Kruit and F. H. Read, *Magnetic field paralleliser for 2π electron-spectrometer and electron-image magnifier*, [J. Phys. E: Scientific Instruments 16 \(1983\) 313-324](#). 

L4. Simulation Laboratory

(Zehra Nur Erengil – ZNE, Gregor Kowarik-GK, Manolis Benis - MB)

L4.1 SIMION TOF modules (ZNE, GK, MU)

L4.2 SIMION TOF modules (ZNE, GK, MU)


L4.3 SIMION TOF modules (ZNE, GK, MU)

L4.4 SIMION TOF modules (MB, ZNE, GK)

L4.5 SIMION TOF modules (MB, ZNE, GK)

L4.6 SIMION TOF modules (MB, ZNE, GK)

Bibliography

- [1] [SIMION 8 manual](#)
- [2] SIMION 8 update Overview - Course Notes 

Program of Lectures and Labs

Unit 4: Time-of-Flight Devices and Mass Analyzers

| Time | Section | Lecturer |
|-----------------------|---------------------------------------|------------------------------|
| Tuesday Sept 6 | | |
| 9:00-10:00 | 4.1 Mass Spectrometry | Hamdi Sukur Kilic |
| 10:00-11:00 | 4.2 Ion Sources | Hamdi Sukur Kilic |
| 11:00-11:30 | Coffee Break | |
| 11:30-12:30 | 4.3 Mass Analysers | Hamdi Sukur Kilic |
| 12:30-13:30 | 4.4 Time-of-Flight Mass Spectrometers | Hamdi Sukur Kilic |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L4.1 SIMION TOF modules | ZN Erengil, M Ulu, G Kowarik |
| 15:30-16:30 | L4.2 SIMION TOF modules | ZN Erengil, M Ulu, G Kowarik |
| 16:30-17:30 | L4.3 SIMION TOF modules | ZN Erengil, M Ulu, G Kowarik |

Wednesday Sept 7

| | | |
|-------------|-------------------------------------------------|-----------------------------------------------------|
| 9:00-10:00 | 4.5 Reflectron TOF Mass Spectrometer | Hamdi Sukur Kilic |
| 10:00-11:00 | 4.6 Important Applications of Mass Spectrometry | Hamdi Sukur Kilic |
| 11:00-11:30 | Coffee break | |
| 11:30-12:30 | 4.7.1 TOF using a Magnetic Bottle | Manolis Benis |
| | 4.7.2 Production of nanosecond pulsed beam | Gregor Kowarik |
| 12:30-13:30 | 4.8 ECTS ACCREDITATION exam on Unit 4 | HS Kilic, ZN Erengil, M Benis, G Kowarik, O Sise |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L4.4 SIMION TOF modules | ZN Erengil, M. Benis, G Kowarik |
| 15:30-16:30 | L4.5 SIMION TOF modules | ZN Erengil, M. Benis, G Kowarik |
| 16:30-17:30 | L4.6 SIMION TOF modules | ZN Erengil, M. Benis, G Kowarik |

Each 1 hour lecture should allow for 10 minutes discussion/questions.

5. Imaging Devices

(Manolis Benis – MB, Fanis Kitsopoulos – FK, Zehra Nur Erengil - ZNE)

5.1 Introduction - Vacuum considerations in imaging devices

(FK)

Basic concepts of vacuum technology and requirements in imaging. Differential pumping. Pulsed valves.

5.2 Velocity Map Imaging (FK)

The principles of VMI spectrometer. Ion imaging. Inverse Abel transformation. Kinematics of DC extraction fields.

5.3 Slice Imaging (FK)

Kinematics of pulsed extraction fields: Slice Imaging. Real-time imaging of ionic fragments. Single field VMI and slice imaging. Resolution effects. Photoelectron detection. Charge particle detection technology.

5.4 Lenses in imaging devices (MB)

VMI with Einzel lens. Low energy photoelectron imaging. Magnification effects. Imaging of the interaction region. Spatial imaging.

5.5 COLTRIMS and Reaction Microscope (MB)

Imaging and coincidence. COLTRIMS: Complete reconstruction of ion kinematics in ionization and fragmentation processes. Coincidences and detection technology involved. Cold gas targets: Jets, Traps (MOTRIMS) and vacuum technology. Detection kinematics. The role of TOF. The Reaction Microscope: COLTRIMS including electron detection. The role of magnetic field. Multi-coincidences.

5.6 Reaction and detection kinematics (MB)

Detailed reaction kinematics. Energy and momentum conservation laws. Examples from fast ion-atom collisions and photoionization. Molecular fragmentation – the axial approximation. Complexity and limitations. Advantages and limitations.




5.7 Case studies of applications of imaging devices (MB)

Examples from applications in molecular ionization and fragmentation

5.8 ECTS accreditation exam on Unit 5 (MB, FK)

Exam on Unit 5 for those participants who have applied for the 6 ECTS units.

Bibliography

- [1] J. Ullrich and V.P. Shevelko (Eds.), [Many-Particle Quantum Dynamics in Atomic and Molecular Fragmentation](#), (Springer-Verlag, Berlin, 2003) pp. 514.
- [2] R. Doerner, V. Mergel, O. Jagutzki, L. Spielberger, J. Ullrich, R. Moshhammer and H. Schmidt-Böcking, *Cold Target Recoil Ion Momentum Spectroscopy: a “momentum microscope” to view atomic collision dynamics*, [Physics Reports 330 \(2000\) 95-192](#). 
- [3] Benjamin Whitaker (Ed.), [Imaging in Molecular Dynamics - Technology and Applications \(A user's guide\)](#) (Cambridge University Press, Cambridge, 2003) pp. 247.
- [4] C Gebhardt, T P Rakitzis, P C Samartzis, V Ladopoulos and T N Kitsopoulos, *Slice Imaging: A New Approach to Ion Imaging and Velocity Mapping*, [Review of Scientific Instruments 72 \(2001\) 3848-3853](#). 
- [5] V. Papadakis and T N Kitsopoulos, *Slice Imaging and Velocity Mapping using a single field*, [Review of Scientific Instruments 77 \(2006\) 083101](#). 

L5. Simulation Laboratory

(Manolis Benis – MB, Fanis Kitsopoulos – FK, Zehra Nur Erengil - ZNE)

L5.1 SIMION modules on Velocity Map Imaging (FK, MB, ZNE)

L5.2 SIMION modules on Slice Imaging (FK, MB, ZNE)

L5.3 SIMION modules on VMI with Einzel lens (FK, MB, ZNE)

L5.4 SIMION modules on interaction volume imaging (MB,ZNE)


L5.5 SIMION modules on COLTRIMS (MB, ZNE)

L5.6 SIMION modules on Reaction Microscope (MB, ZNE)

SIMION final examination SIMION final exam

Certificate diploma and Awards - Evaluations Participation certificate and best student (grade) and most active student awards. Complete evaluation sheets.

Bibliography

- [1] [SIMION 8 manual](#)
- [2] SIMION 8 update Overview - Course Notes 

Program of Lectures and Labs

Unit 5: Imaging devices

| Time | Section | Lecturer |
|------------------------|------------------------------------------------------------------------------------------------|---------------------------------|
| Thursday Sept 8 | | |
| 9:00-10:00 | 5.1 Introduction - Vacuum considerations in imaging devices | Fanis Kitsopoulos |
| 10:00-11:00 | 5.2 Velocity Map Imaging | Fanis Kitsopoulos |
| 11:00-11:30 | Coffee Break | |
| 11:30-12:30 | 5.3 Slice Imaging | Fanis Kitsopoulos |
| 12:30-13:30 | 5.4 Lenses in imaging devices | Manolis Benis |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L5.1 SIMION modules on Velocity Map Imaging | M. Benis, F. Kitsopoulos, |
| 15:30-16:30 | L5.2 SIMION modules on Slice Imaging | M. Benis, F. Kitsopoulos |
| 16:30-17:30 | L5.3 SIMION modules on VMI with Einzel lens | M. Benis, F. Kitsopoulos |
| Friday Sept 9 | | |
| 9:00-10:00 | 5.5 COLTRIMS and Reaction Microscope | M. Benis |
| 10:00-11:00 | 5.6 Reaction and detection kinematics | M. Benis |
| 11:00-11:30 | Coffee break | |
| 11:30-12:30 | 5.7 Case studies of applications of imaging devices | M Benis |
| 12:30-13:30 | 5.8 ECTS ACCREDITATION exam on Unit 5 | M Benis, F Kitsopoulos, M Dogan |
| 13:30-14:30 | Lunch | |
| 14:30-15:30 | L5.4-5.6 SIMION modules on interaction volume imaging, COLTRIMS and Reaction Microscope | M. Benis, ZN Erengil |
| 15:30-16:30 | SIMION final exam | M. Benis, ZN Erengil |
| 16:30-17:30 | Certificate diploma and Awards - Evaluations | All participants |

Each 1 hour lecture should allow for 10 minutes discussion/questions.

CPOTS2011 Instructors teaching Schedule

| Instructor Name | Lectures #unit.section | Labs Sect # | Exams Sect # | Lectures hours | Exams hours | Labs hours | Total hours | GTotal hours |
|-------------------------|------------------------|-------------|--------------|----------------|-------------|------------|-------------|--------------|
| Theo Zouros | #1: - | L1.1-1.3 | | 0 | 0 | 3 | 3 | 16 |
| | #3: 3.1,3.2,3.3 | L3.1-3.6 | 3.8 | 3 | 1 | 6 | 10 | |
| | #5: - | L5.4-5.6 | | 0 | 0 | 3 | 3 | |
| Fanis Kitsopoulos | #5: 5.1,5.2,5.3, 5.7 | L5.1-5.3 | 5.8 | 4 | 1 | 3 | 8 | 8 |
| Genoveva Martinez-Lopez | #1: 1.1-1.3, 1.4, 1.7 | - | 1.8 | 5 | 1 | 0 | 6 | 8 |
| | #2: | - | 2.8 | 0 | 1 | 0 | 1 | |
| | #3: | - | 3.8 | 0 | 1 | 0 | 1 | |
| Mevlut Dogan | #2: 2.4 | L2.1-2.6 | 2.8 | 1 | 1 | 6 | 8 | 10 |
| | #3: | - | 3.8 | 0 | 1 | 0 | 1 | |
| | #5: | - | 5.8 | 0 | 1 | 0 | 1 | |
| Melike Ulu | #1: - | L1.4-1.6 | - | 0 | 0 | 3 | 3 | 17 |
| | #2: 2.1 | L2.1-2.6 | 2.8 | 1 | 1 | 6 | 8 | |
| | #4: - | L4.1-4.6 | - | 0 | 0 | 6 | 6 | |
| Omer Sise | #1: - | L1.1-1.6 | - | 0 | 0 | 6 | 6 | 17 |
| | #2: 2.2,2.3,2.7 | L2.1-2.6 | 2.8 | 3 | 1 | 6 | 10 | |
| | #4: | - | 4.8 | | 1 | 0 | 1 | |
| Zehra Nur Erengil | #2: - | L2.1-2.6 | - | 0 | 0 | 6 | 6 | 15 |
| | #4: - | L4.1-4.6 | - | 0 | 0 | 6 | 6 | |
| | #5: - | L5.4-5.6 | - | 0 | 0 | 3 | 3 | |
| Hamdi Sukur Kilic | #1: | - | 1.8 | 0 | 1 | 0 | 1 | 11 |
| | #2: | - | 2.8 | 0 | 1 | 0 | 1 | |
| | #4: 4.1-4.6 | L4.4-4.6 | 4.8 | 6 | 1 | 3 | 9 | |
| Gregor Kowarik | #1: - | L1.4-1.6 | - | 0 | 0 | 3 | 3 | 17 |
| | #3: - | L3.1-3.6 | - | 0 | 0 | 6 | 6 | |

| | #4: 4.7 | L4.1-4.6 | 4.8 | 1 | 1 | 6 | 8 | |
|----------------------|-------------------|----------|-----|---|---|---|----|-----------|
| Manolis Benis | #1: - | L1.1-1.3 | - | 0 | 0 | 3 | 3 | 20 |
| | #4: 4.7 | L4.4-4.6 | 4.8 | 1 | 1 | 3 | 5 | |
| | #5.1,5.4-5.7 | L5.1-5.6 | 5.8 | 5 | 1 | 6 | 12 | |
| Nikos Tsoupas | #1: 1.4 -1.6 | - | 1.8 | 3 | 1 | 0 | 4 | 19 |
| | #2: 2.5 -2.7 | - | 2.8 | 3 | 1 | 0 | 4 | |
| | #3: 3.3, 3.5 -3.7 | L3.1-3.6 | 3.8 | 4 | 1 | 6 | 11 | |