CHARGED PARTICLE OPTICS – THEORY AND SIMULATION (CPOTS)

Erasmus Intensive Programme

Physics Department University of Crete

August 15 – 31, 2013

Heraklion, Crete, Greece

Participating Institutions and Instructors

1. University of Crete (UoC)
    - **Prof. Theo Zouros* (Project coordinator)**
2. Afyon Kocatepe University (AKU)
    - **Prof. Mevlut Dogan** (contact)
    - Dr. Zehra Nur Özer*
3. Selçuk University (SU)
    - **Prof. Hamdi Sukur Kilic** (contact)
4. Universidad Computense Madrid (UCM)
    - **Prof. Genoveva Martinez - Lopez** (contact)
    - Pilar Garcés*
5. University of Ioannina (UoI)
    - **Prof. Manolis Benis*** (contact)
6. Technische Universität Wien (TUW)
    - **Prof. Christoph Lemell***
7. Queen's University Belfast (QUB)
    - **Prof. Jason Greenwood*** (contact)
    - Louise Belshaw*
8. University of Debrecen (UoD)
    - **Prof. Béla Sulik** (contact)
9. University of Athens (UoA)
    - **Prof. Theo Mertzimekis** (contact – was not able to be present)

*SIMION user

Medical University of South Carolina

- **Prof. Dan Knapp** (guest)

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 + lab hours at an Erasmus IP: **5 hours**(as certified by the attendance sheet).
3. A minimum of two 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.
5. Teacher advisors will be assigned to each project group to help out where needed.

Students

1. A CPOTS2013 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 awarded to all students with the CPOTS2013 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 will have 4 exams one for each of the 4 Units of the IP, a comprehensive SIMION final exam and a group project presentation. Each Unit exam will be given at the end of each unit as indicated in the work program, while the project presentation and SIMION final will be on the last day of the IP.
4. The overall course grade will be determined as follows:
   40% from the average of the 4 Unit exams, 25% from the SIMION final exam, 25% from the Project presentation grade and 10% from overall class participation.
5. All student participants <u>must take all the exams</u> even if not interested in the 6 ECTS.

1. Transport of Charged Particle Beams

(Genoveva Martinez Lopez – GML, Christoph Lemell – CL)

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 Calculation of charged particle trajectories – numerical methods *(GML)*

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

1.3 Monte-Carlo simulations *(CL)*

Motivation: realistic modeling of beam transport. Introduction to Monte-Carlo technique. Random-number generators. Distributions of random numbers. Generating an ensemble of test particles.

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

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

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

1.5 Gaussian Optics *(GML)*

Ideal imaging properties of electrostatic systems. Fundamental rays. Cardinal points. Ideal imaging properties of magnetostatic systems. The equation of motion in fixed and rotating axes.

1.6 Phase Space, Beam Emittance and the Liouville theorem *(CL)*

Motivation: statistical description of systems. Hamiltonian mechanics. Phase space. Liouville's theorem. Emittance, acceptance. Solving Liouville's equation.

1.7 Transfer Matrices and First-Order Beam Transport *(CL)*

Motivation: obtain estimate for charge transport. Concept of transfer matrices. Transfer matrices for simple systems.

1.8 ECTS accreditation exam on Unit 1 *(GML+CL)*

Exam on Unit 1 for all student participants.

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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[9] S. Y. Lee, *Accelerator Physics*, (World Scientific, 1999).

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[15] Karl L. Brown, *A First- and Second-Order Matrix Theory for the Design of Beam Transport Systems and Charged Particle Spectrometers*, SLAC Report-75, 1982

[16] J. Buon, *Beam Phase Space and Emittance*, http://cours.lal.in2p3.fr/ecoles/accelerateurs/Jbuon2.pdf

[17] S. Saminathan, *Extraction and transport of ion beams from an ECR ion source*, PhD thesis Rijksuniversiteit Groningen

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2. Focusing Systems – Lenses – Ion Traps

(Mevlut Dogan – MD, Zehra Nur Özer – ZNO, Genoveva Martinez Lopez – GML, Jason Greenwood - JG)

2.1 Introduction to Focusing Devices and Electrostatic Lenses *(MD)*

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 Aberrations in CPO *(GML)*

Ideal imaging. Geometrical aberrations of electron optics imaging systems: aberration figures. Chromatic and asymmetric aberrations.

APPENDIX: General scheme for the calculation of aberrations.

2.3 Focal and Zoom Lens Properties *(MD)*

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.

2.4 Case Studies of Electrostatic Lenses – Applications *(MD)*

Three-Element Lenses. Four-Element Lenses. Five-Element Lenses. Electron guns. Entrance optics of energy analyzers. Other examples

2.5 Magnetic Lenses + Sector Field Lenses *(JG)*

Basic Principles. Advantages of Magnetic Lenses. Lorentz Force. Types of magnetic fields and their generation. Different Lenses. Simple Solenoid lens. Magnetic Sector Lens. Quadrupole Lens

2.6 Ion Traps *(JG)*

Introduction. Why Traps? Mass dependent motion in conservative fields, Earnshaw's theorem, Types of Ion Traps, RF Devices/Paul Trap, Penning Trap, Kingdon Trap, Orbitrap, Linear Electrostatic Trap (LEIT).

2.7 ECTS accreditation exam on Unit 2 *(MD+GML+JG)*

Exam on Unit 2 for all student participants.

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.

[3] Jon Orloff, Handbook of Charged Particle Optics, 2nd edition (CRC Press, Rockaway Beach, Oregon, USA, 2008) pp. 666

[4] P. Grivet, Electron Optics, Pergamon Press, London, 1965.

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3. Energy and Momentum Dispersion Analyzers

(Béla Sulik – BS, Theo Zouros-TZ)

1.1 Charged Particle Dispersion Analyzers *(BS)*

Typical spectroscopy -light (traditional concepts) and particles. Charge particle spectra - Auger, continuum. Energy dispersion-momentum dispersion-time of flight. Spectroscopy versus spectrography. Simple spectrometers - dispersion and resolution. Traditional optical parameters - versus simulations. Collision experiments, cross section. Some examples - simple and complicated spectrometer systems. Magnetic spectrographs

3.2 Electrostatic Spectrometers: Basic Operation *(TZ)*

Example of complete system: The 0^0 projectile e- spectrometer. Basic components of a complete spectrometer. Difference between a lens and a dispersion analyzer. Dispersion analyzer – Optics. Dispersion Analyzer Spectrum recording modes. Examples: The 45^0 Parallel Plate Analyzer (PPA). Spectrographic mode: Use of position sensitive detector to define energy. Examples: The HDA spectrograph - voltage and DAQ electronics

Appendix I: The trajectory of a PPA – focusing properties

3.3 Electrostatic Spectrometers: Energy Resolution and Focusing Properties *(TZ)*

Energy resolution and Base width of an Analyzer. Derivation of the Base Energy resolution of a 45^0 PPA. The trace width. General formula for energy resolution of all dispersion analyzers. Different types of Analyzers – focusing properties. The hemispherical deflector analyzer (SDA). Improving the energy resolution by pre-retardation

3.4 Momentum Dispersion and Magnetic Spectrometers *(BS)*

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

3.5 Particle Detectors and Electronics *(BS)*

Various types of particle detectors. Channeltron and Channel plate detectors. 1-D and 2-D position sensitive detectors. Preamplifiers. Amplifiers. Pulse shaping electronics. Analog to digital converters. Digital to Analog converters. Time Digital converters.

3.6 *ECTS* accreditation exam on Unit 3 (BS+TZ)

Exam on Unit 3 for all student participants.

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] B John H. Moore, Christopher C. Davis, Michael A. Coplan and Sandra C. Greer, *Building Scientific Apparatus*, 4rth edition (Cambridge University Press, July 20, 2009), pp. 662.

[3] K. D. Sevier, *Low Energy Electron Spectrometry*, (Wiley, New York, 1972).

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4. TOF, Mass Spectrometry and Imaging

(Hamdi Sukur Kilic – HSK, Manolis Benis –MB, Dan Knapp - DK)

4.1 Introduction to Mass Spectrometry and Molecular Ion Sources *(DK)*

Introduction Mass Spectrometry, Identification Components of Mass Spectrometry, What is ION?, Resolution of a Mass Spectrometry, Production of a Mass Spectrum, Interpretation of The Mass Spectra, Application of Mass Spectrometry

4.2 TOF and Re-TOF Mass Spectrometry *(HSK)*

Introduction TOF-MS, Main Components of TOF-MS, Focusing and Resolution Process, Basic Principle of TOF-MS, Calibration of The m/q Scale. Introduction Re-ToF-MS, A Comparison of Re-ToF-MS and Linear ToF-MS, Matrix-Assisted Laser Desorption Ionization (MALDI), Sample Preparation for MALDI, MALDI Matrix.

4.3 Velocity Mapping and Slice Imaging, COLTRIMS and Reaction Microscopes *(MB)*

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

4.4 Proteomics and Tandem Mass Spectrometry *(DK)*

Proteomics: what is it, why do it, how it is done. Tandem mass spectrometry. Fragmentation of peptides. Identification of proteins. Quantitation of protein expression.

4.5 ECTS accreditation exam on unit 4 *(HSK+MB+JG+DK)*

Exam on Unit 4 for all student participants.

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.

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S. SIMION 8.1 workshop

(Theo Zouros – TZ, Manolis Benis –MB, Jason Greenwood – JG, Christoph Lemell - CL)

S.1 Introduction to SIMION 8.1 *(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.

S.2 Building the electrodes - Modifying PA geometries *(MB)*

S.3 Building the electrodes - Modifying PA geometries (continued) *(MB)*

Creating Potential Arrays in SIMION. The Modify function/environment. A how-to-build approach. The Modify Viewing Interface

S.4 Solving Laplace's Equation: Loading, Saving, Refining and Fast Adjusting PAs *(JG)*

The SIMION potential array. Solving the Laplace Equation. Refining potential arrays. Fast Adjusting Electrodes

S.5 Creating a Workbench – Positioning and Viewing PAs *(MB)*

The concept of Ion Optics Workbench. Positioning Potential Arrays in Workbench. Viewing Potential Arrays in Workbench. Workbench in details

S.6 Defining, Flying and Recording Particles *(TZ)*

Ion Definitions, Defining Ions in Groups (.FLY, .FLY2), Defining Ions Individually (.ION)
Defining Ions Outside of SIMION (.ION),

S.7 Defining, Flying and Recording Particles (continued) *(TZ)*

Data Recording (.REC), Data Recording to a File, What, When, How, and Where to record, Using the Data Monitoring Screen, Recording Trajectories (.TRJ)

S.8 User modifications of SIMION: Lua and the workbench *(CL)*

S.9 User modifications of SIMION: Lua and the workbench (continued) *(CL)*

Why learning a new computer language? Concepts of user interaction with SIMION. Startup scripts. Command-line interaction. Batch programs. Workbench programs. Introduction to Lua. A simple example of workbench programming

S.10 Introduction to building PAs from Geometry files *(MB)*

Creating Potential Arrays in SIMION. The Geometry function/environment. A how-to-build approach. The Viewing Interface. Classes of Instructions. Structure of most commonly used instructions. The nesting rules.

S.11 Building PAs from Geometry files - Examples (MB)

Geometry Language Rules & Instructions. Example 1: Creating a union cross. Example 2: Creating a cone. Creating a hollow cone. Example 3: Creating uniform magnetic field. Example 4: Working with dummy variables (SIMION 8.1). Example 5: Creating a sinusoidal shaped surface.

S.12 Magnetic Pas – Using Magnetic Fields in SIMION *(JG)*

Treating Magnetic Fields in SIMION. Magnetic Scalar Potential. User Calculated Fields. Limitations / Future Developments. Simple Magnetic Field Examples. Uniform Field. Magnetic Sector. Solenoid / Helmholtz Coils. Displaying field lines

Bibliography

[1] A fairly complete list of useful reading material and examples can be found at: SIMION_course_material.php

[2] Another important source for all SIMION is the **Help> SIMION 8.1 Supplemental Documentation** in SIMION itself (Help on SIMION Windows title bar)

[3] Geometry Files (GEM files):

- SIMION 8.1 Manual: Appendix I - Geometry Files (GEM Files)
- GEM Geometry files in SIMION 8.1
- Anisotropically Scaled Grid Cells in SIMION 8.1

AS. Advanced SIMION 8.1 workshop

(Theo Zouros – TZ, Manolis Benis –MB, Jason Greenwood – JG, Christoph Lemell – CL, Giannis Gennarakis* – GG, Tobias Bauer* - TB)

AS1. The Lua Programming language *(CL)*

Further language elements. Modules and packages. Contents of some libraries (Lua and SIMION). Some example(s)

AS2. Workbench User Programming *(CL)*

The Flow diagram of Fly'm. Possibilities of user interaction. Simion work bench segments.

AS3. Workbench User Programming – Examples *(CL)*

Possibilities of user interaction. Example: Simulation of the Franck-Hertz experiment in SIMION

AS4. Accuracy in (SIMION) simulations *(TZ)*

Some nice new features in SIMION 8.1. Accuracy in SIMION simulations. How accurate are my SIMION results!??? How to check SIMION accuracy? Use a system with analytical closed form trajectories. The Spherical Capacitor (SC). Potential in a SC. Motion in an SC. SC Gem files. The coarseness of the SC electrodes in SIMION. Results for circular orbits in an SC. Conclusions about accuracy of SIMION trajectories in SC. Errors in geometry simulations. Surface enhancement. Reminder: Differences between Modify and View Screens. Further capabilities with surface enhancement. Definition of pa_define command. More "professional" version of example Einzel_param.gem

AS5. Using STL files with SIMION (GG)

Introduction to the STL Files. Basic Operations in Solidworks. Design of a 5-element lens in Solidworks. Importing STL parts into SIMION. Creating a lens through a geometry file. Refining and Importing parts into the workbench. Flying particles. Analyzing Results

AS6. Electrons trajectories in a Laser Field *(JG)*

Nature of intense laser fields. Free electron motion in oscillating E field. Electron re-collision in atoms. Influence of B field at relativistic intensities. Simulation of Intense Laser field in SIMION.

AS7. Complete examples using GEM files and User Programs *(TB)*

The WalThemis Experimental Setup at Univ. of Frankfurt and its SIMION simulation. Example of SIMION batch mode usage.

*CPOTS Student contributions

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[1] A fairly complete list of useful reading material and examples can be found at: SIMION_course_material.php

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