Course Informations

CH1: Drug Discovery

Time: 20.-24.8.2012
Credits: 3 ECTS
Lectures: 20 h lectures and exam
Coordinators: Juhani Huuskonen and Olli Pentikäinen
Lecturers: Martin Bauer (AstraZeneca, Sweden), Erik Wallén (Univ. Helsinki, Finland), Adyary Fallarero (Åbo Akademi University, Finland), Jay Pandit (Pfizer,USA), John Overington (EBI/EMBL,UK) and Olli Pentikäinen (University of Jyväskylä)
Prerequisites: M.Sc. or equivalent in Chemistry, Biochemistry, or Pharmacy, or related. M.Sc. students in their final term in one of the subjects are encouraged to apply as well.
Passing: Obligatory attendance at lectures and written examination
Grading: Pass/fail
Abstract: This course introduces the key methods in drug discovery, including, but not limited to: measurements of biological activity; high-throughput screening; computer-aided molecular discovery; virtual high-throughput screening; structural studies of proteins, ligands, and their complexes; organic synthesis.

CH3: The Physics and Chemistry of Atomic Clusters

Time: 13.–24.8.2012
Lectures: 20 h + homework
Credits: 3 ECTS
Coordinator: Prof. Hannu Häkkinen
Lecturers: Prof. Henrik Grönbeck (Chalmers University of Technology, Sweden) and Prof. Hannu Häkkinen (JYU)
Prerequisites: The course is suited for graduate or last year under-graduate students.
Passing: Obligatory attendance to lectures and homework
Abstract: Atomic clusters, with sizes from a few to thousands of atoms, represent a fascinating cross-disciplinary field of research on the border between chemistry, physics and materials science. Clusters can be formed from virtually any element in the Periodic Table and are most often characterized according to the types of bonding being covalent, metallic or van der Waals. Because of their finite size, clusters often show properties that are markedly different with the corresponding bulk property. Illustrative examples are the discoveries of electronic shell closings for metallic clusters and C_{60} for carbon clusters. Thanks to novel properties, nano-structuring in the form of clusters open up new routes for materials design. This course will give an introduction to atomic clusters, describe common methods used to investigate clusters experimentally and theoretically, and highlight present and future applications.

The course will:

- Introduce the field of clusters

- Discuss different types of clusters
- Describe methods used in cluster research
- Describe chemical and physical properties of clusters
- Discuss present challenges within cluster research
- Discuss technical applications of clusters

The course will have ten two-hour lectures centered around:

1) Phenomenological description of clusters
2) Experimental methods to fabricate and study clusters
3) Theoretical methods used to study clusters
4) Electronic properties
5) Structural motifs
6) Thermodynamic properties
7) Chemical properties
8) Ligand stabilized clusters
9) Supported clusters
10) Applications of clusters

COM4: Evolutionary Optimisation of Expensive Problems

Time: 13.–17.8.2012
Lectures: 15 hours of lectures, 3 hours of assignments and 2 hour exam
Credits: 2 ECTS
Maximum of Students: 24
Coordinators: Jussi Hakanen and Kaisa Miettinen
Lecturer: Yaochu Jin
Prerequisites: Good knowledge in linear algebra and calculus required.
Passing: Obligatory attendance at lectures, assignments (60%) and exam (40%).
Grading: 1-5
Abstract: This course aims to provide hands-on skills and up-to-date knowledge on evolutionary optimisation of expensive problems. The course begins with an introduction to traditional optimisation methods such as the Simplex method and gradient based methods. Then, fundamental evolutionary algorithms, including genetic algorithms, evolution strategies particle swarm optimisation will be discussed. Techniques for building linear and nonlinear models (surrogates), such as artificial neural networks will be presented. Memetic algorithms, which combine evolutionary search and local search techniques will also be discussed. Dynamic weighted aggregation methods, non-dominated crowded sorting genetic algorithms and a regularity based estimation of distribution algorithms for multi-objective optimisation techniques will be presented. Based on the above, surrogate-assisted evolutionary algorithms for dealing with expensive optimisation problems will be given. Fundamental model management techniques, including individual based, generation based and population based methods,

will be introduced. Use of surrogates in memetic algorithm in combination with the trust region method will be given. Finally, advanced topics in surrogate-assisted evolutionary optimisation of expensive problems will be discussed and real-world examples will be given to shown how the techniques described in this course can be employed.

MA3: Markov Chain Stability and Applications

Time: 13.–17.8.2012
Place: MaD202
Lectures: 10 h lectures and 6 h demonstrations
Credits: 2 ECTS
Coordinator: Matti Vihola
Lecturer: Eric Moulines
Prerequisites: A first course with measure theoretical probability theory (e.g. Billingsley: Probability and measure, Chung: A course in probability theory). Some insights on martingales and discrete state space Markov chains are useful but not necessary.
Passing: Obligatory attendance at lectures.
Grading: Pass/fail
Abstract: This course will provide an introduction to the theory and applications of Markov chains over general state spaces. The course will start from the basics in Markov chains and then, using many examples taken from dynamical systems and from Monte Carlo methods, will gradually introduce some of the main modern concepts underlying the theory of Markov chains over general state space.