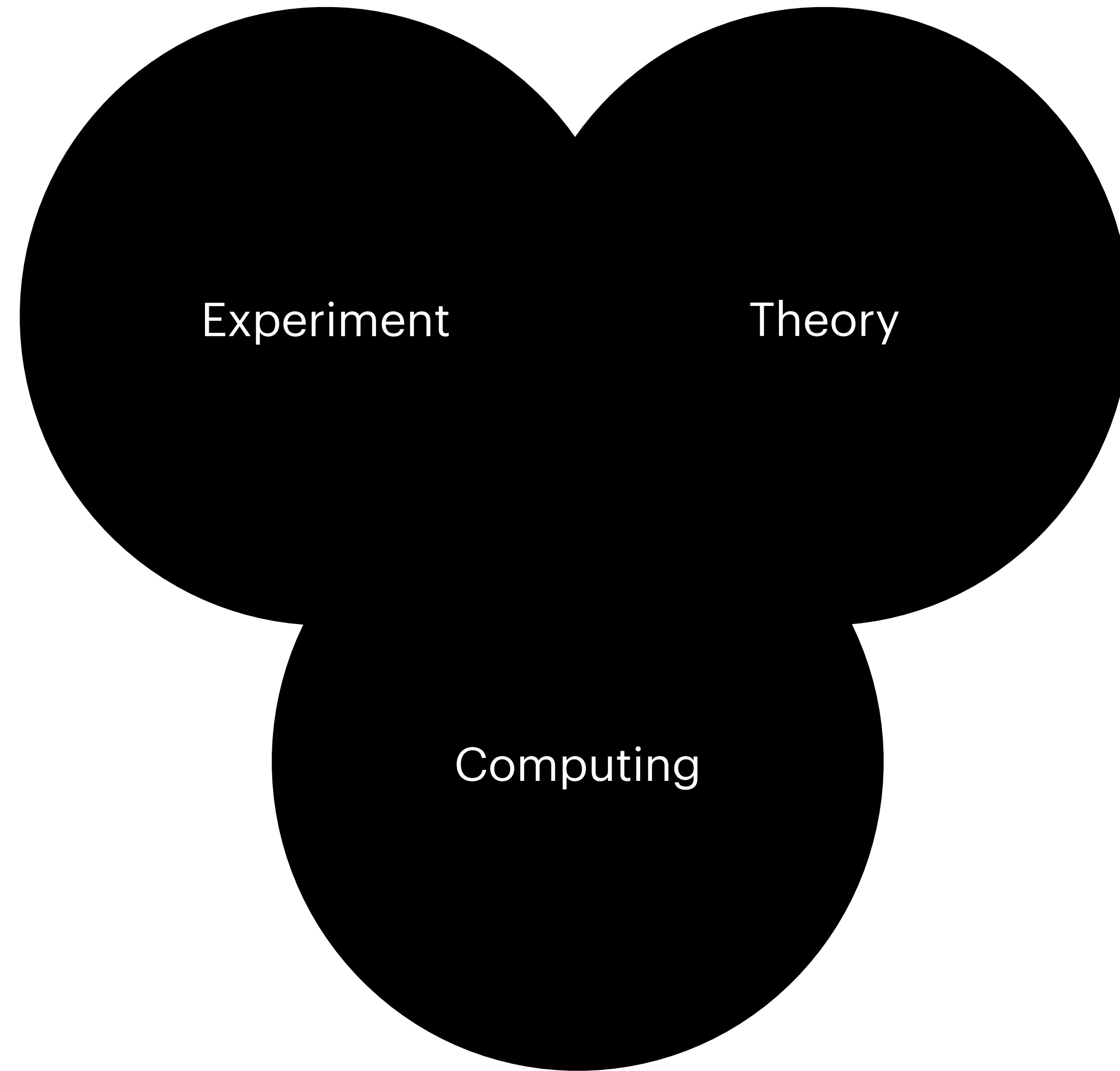


Computational Science and Engineering - Specialisation in Theoretical Physics

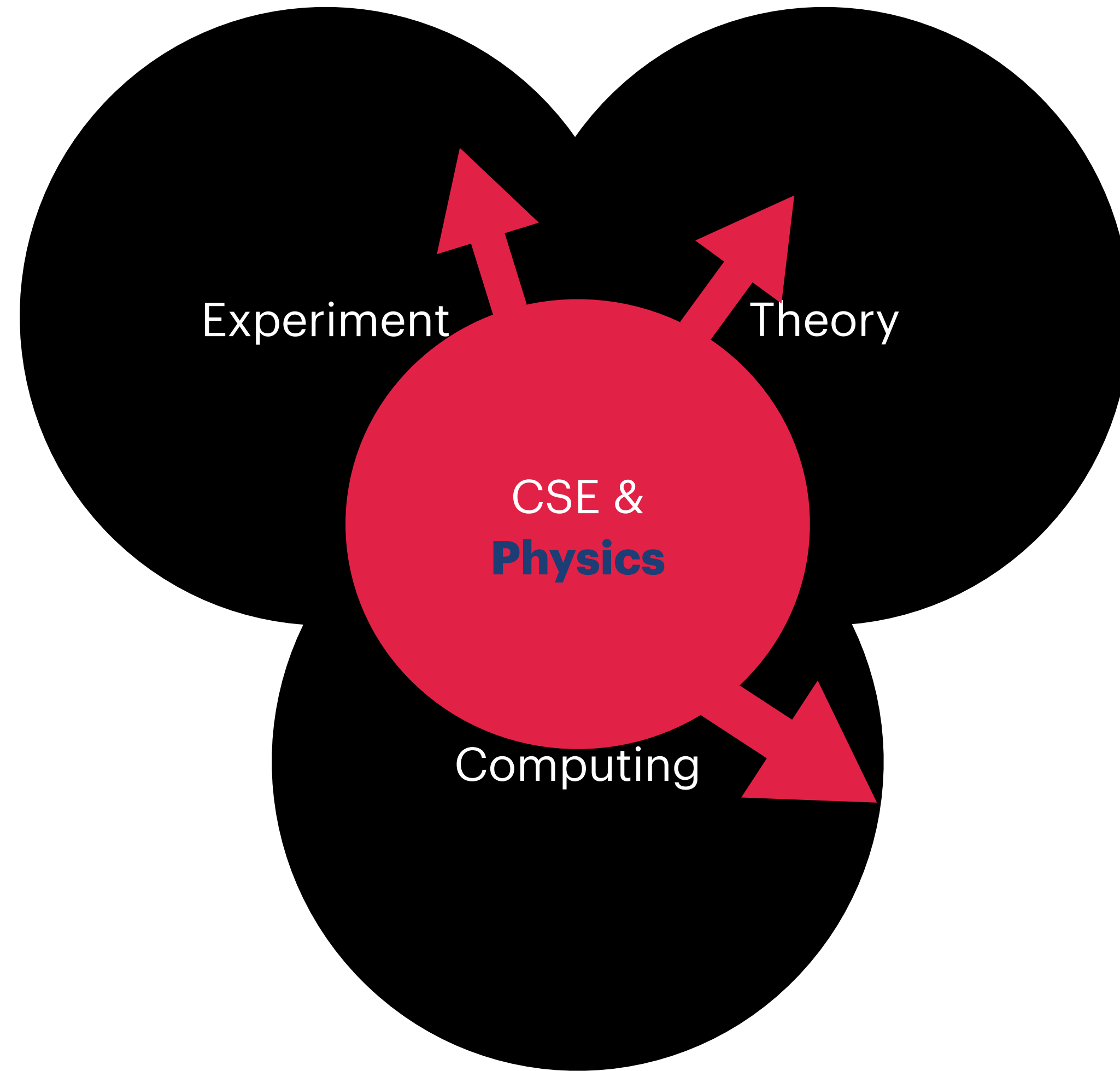
Andreas Adelmann

May 2020

The 3 legs of science

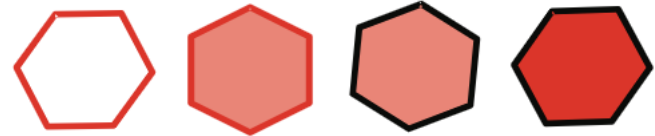


The 3 legs of science **and you are in the middle**



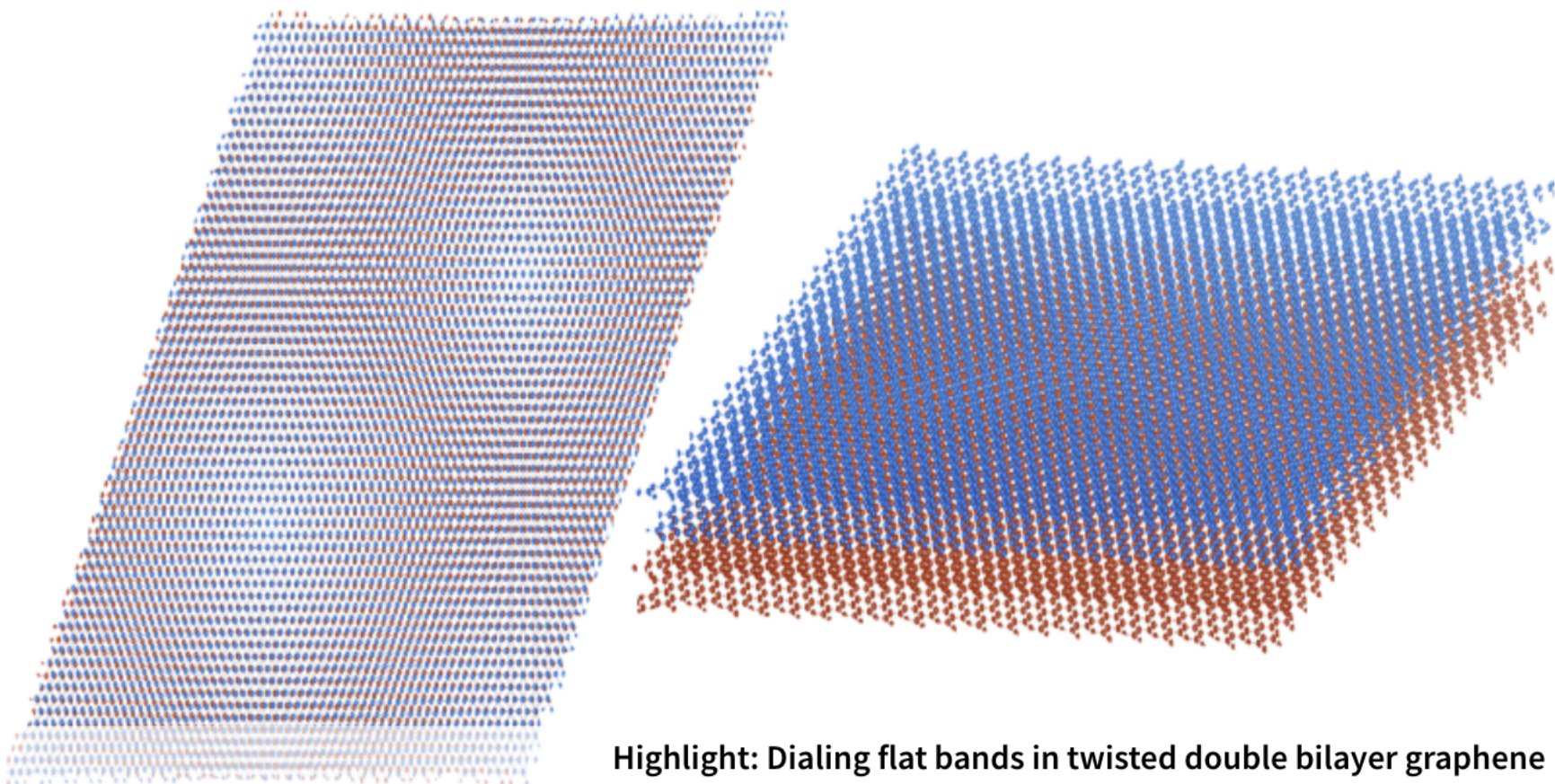
The 3 legs of science **and you are in the middle**

MARVEL

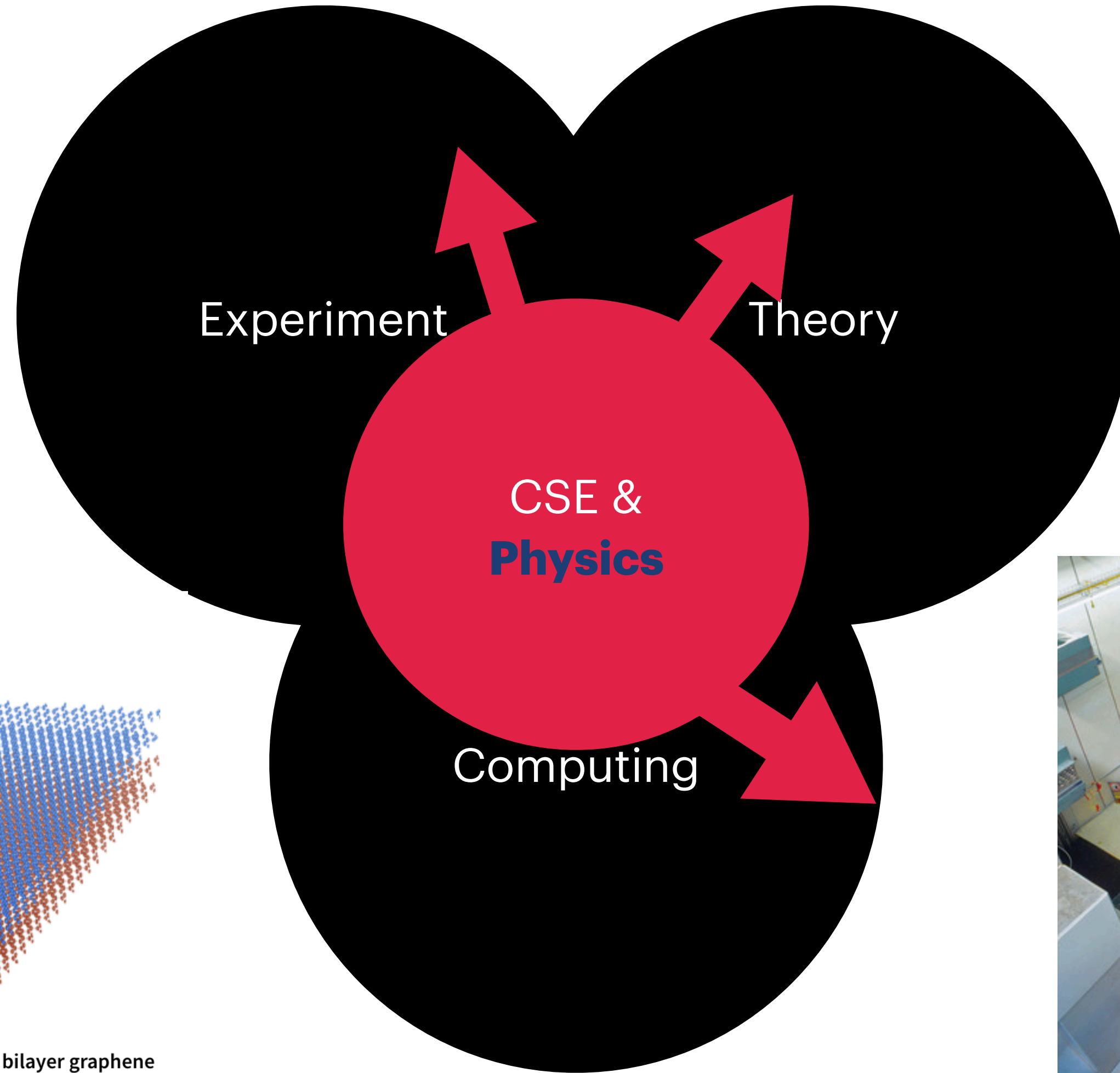


NATIONAL CENTRE OF COMPETENCE IN RESEARCH

MARVEL is a centre on
**Computational Design
and Discovery of Novel
Materials**



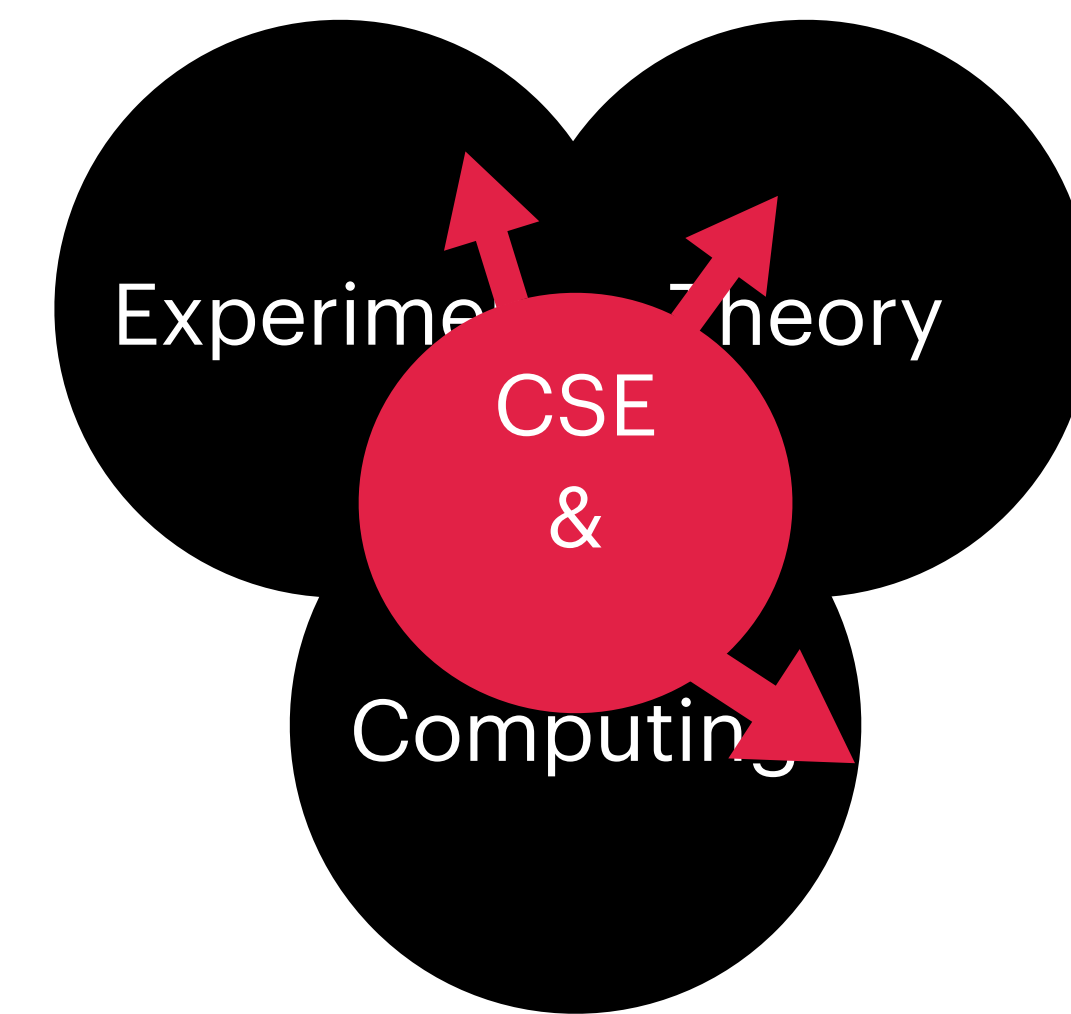
Highlight: Dialing flat bands in twisted double bilayer graphene



Center for Proton Therapy CPT (PSI)



What are the challenges ?



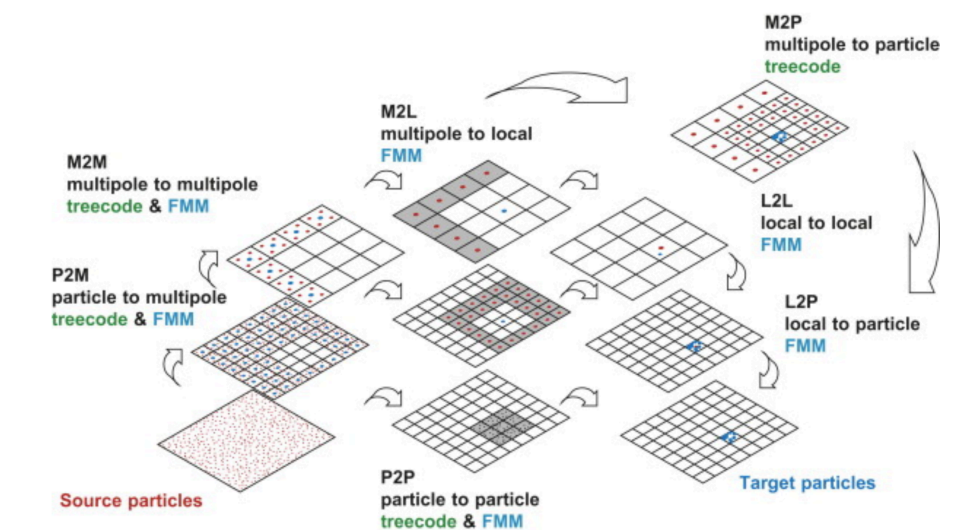
★ Models from theory are too complex for an **analytic** solution

-> almost all interesting physics problems



★ Algorithms are too complex to compute a solution in a **reasonable** time

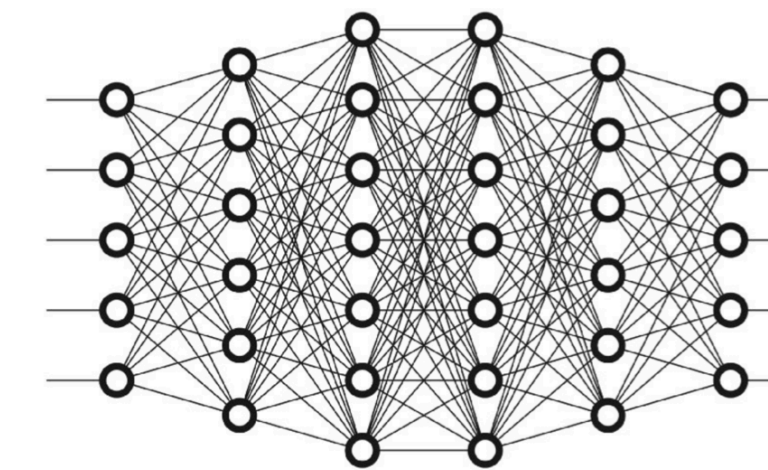
-> n-body problems



<https://www.sciencedirect.com/science/article/pii/B9780123849885000097#f0010>

★ Data are too complex in structure and **large in size**

-> LHC > 2PB are being accessed (RW) every day



In the CSE curriculum so far you learned all the necessary **skills, tools and methods to become a Computational Physicist**

Curriculum

Introduction to Computational Physics

Methods for physics problems and their implementation

(classical equations of motion, partial differential equations, Monte Carlo simulations, phase transitions, percolation...)

Computational Statistical Physics

Computer simulation methods in (classical) statistical physics

(e.g. Monte Carlo methods, Molecular dynamics, parallelization, ...)

Computational Quantum Physics

Simulation methods for quantum systems (incl. quantum many-body systems)

(e.g. Quantum Monte Carlo, Density Functional theory, Hartree Fock, exact diagonalisation, ...)

Molecular and Materials Modelling

Basic techniques to interpret experiments with contemporary atomistic simulation

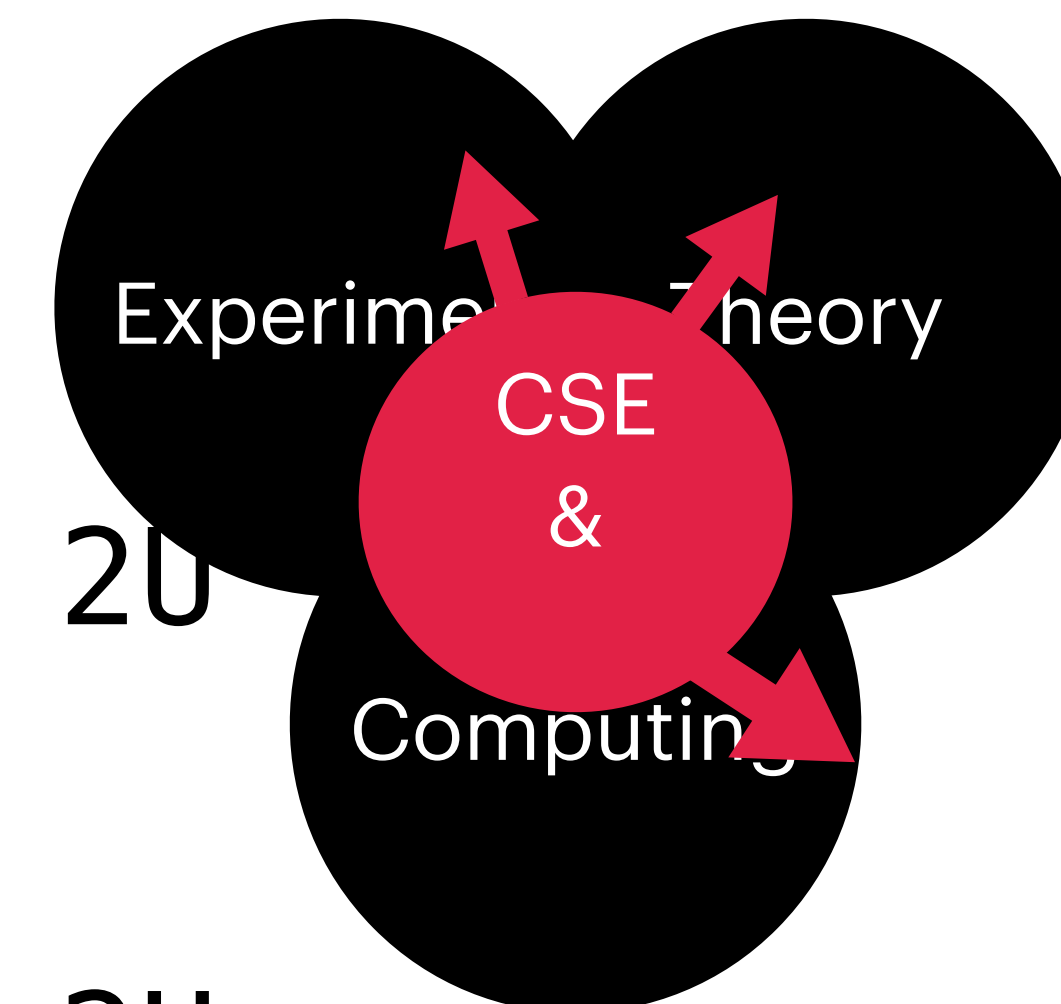
(e.g. ab-initio based molecular dynamics, Monte Carlo, Big Data, hands-on for realistic systems)

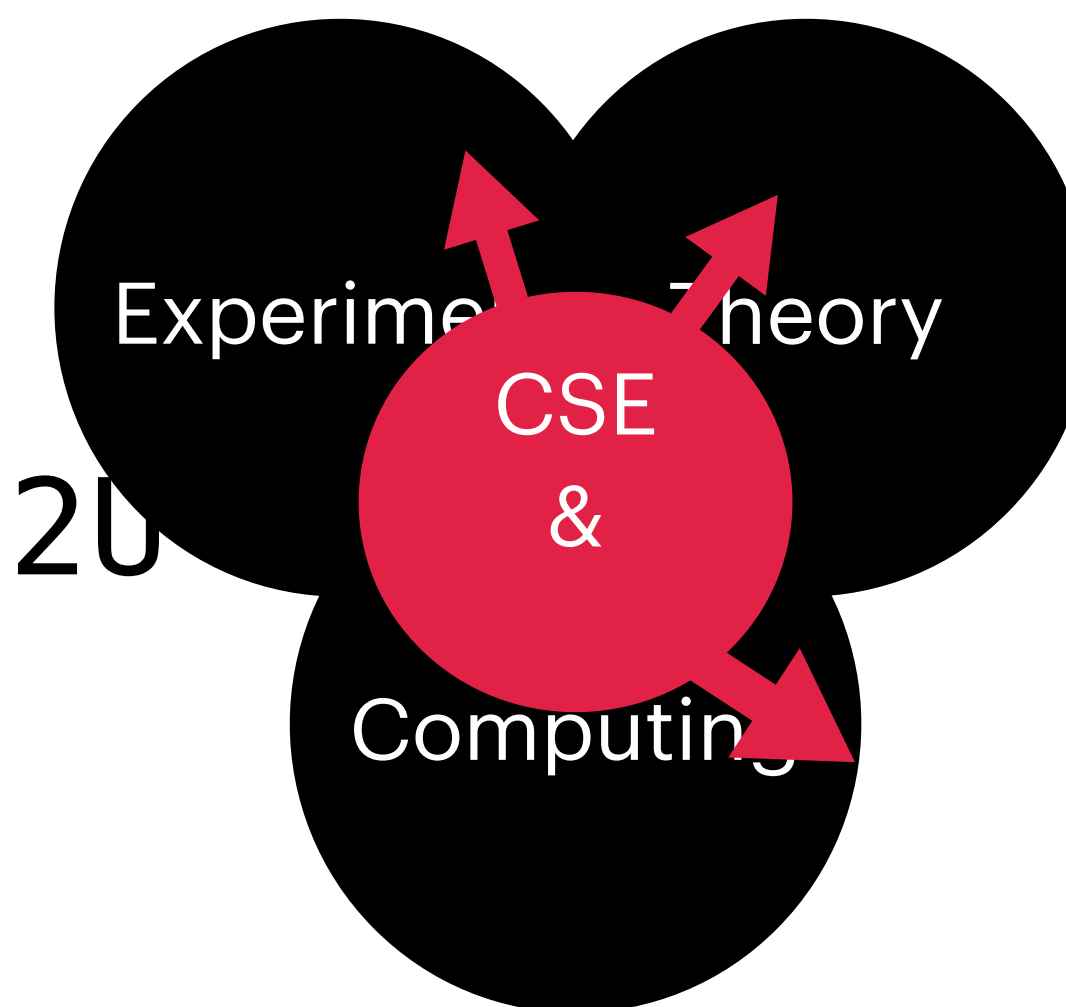
2V 2U

2V 2U

2V 2U

2V 2U





Quantenmechanik I

Einführung in die Quantentheorie: Wellenmechanik, Schroedingergleichung, Drehimpuls, Spin, Struktur der Quantentheorie: Hilbertraeume, Zustände und Observable, Bewegungsgleichung

3V 2U

Quantenchemie

Einführung in Konzepte der Elektronenstruktur-Theorie und in die Methoden der numerischen Quantenchemie

3G

Quantum Information Theory

Introduce the foundations of quantum information theory, introduction to the mathematical theory of information, basic information-theoretic aspects of quantum mechanics, applications such as quantum cryptography and quantum computing.

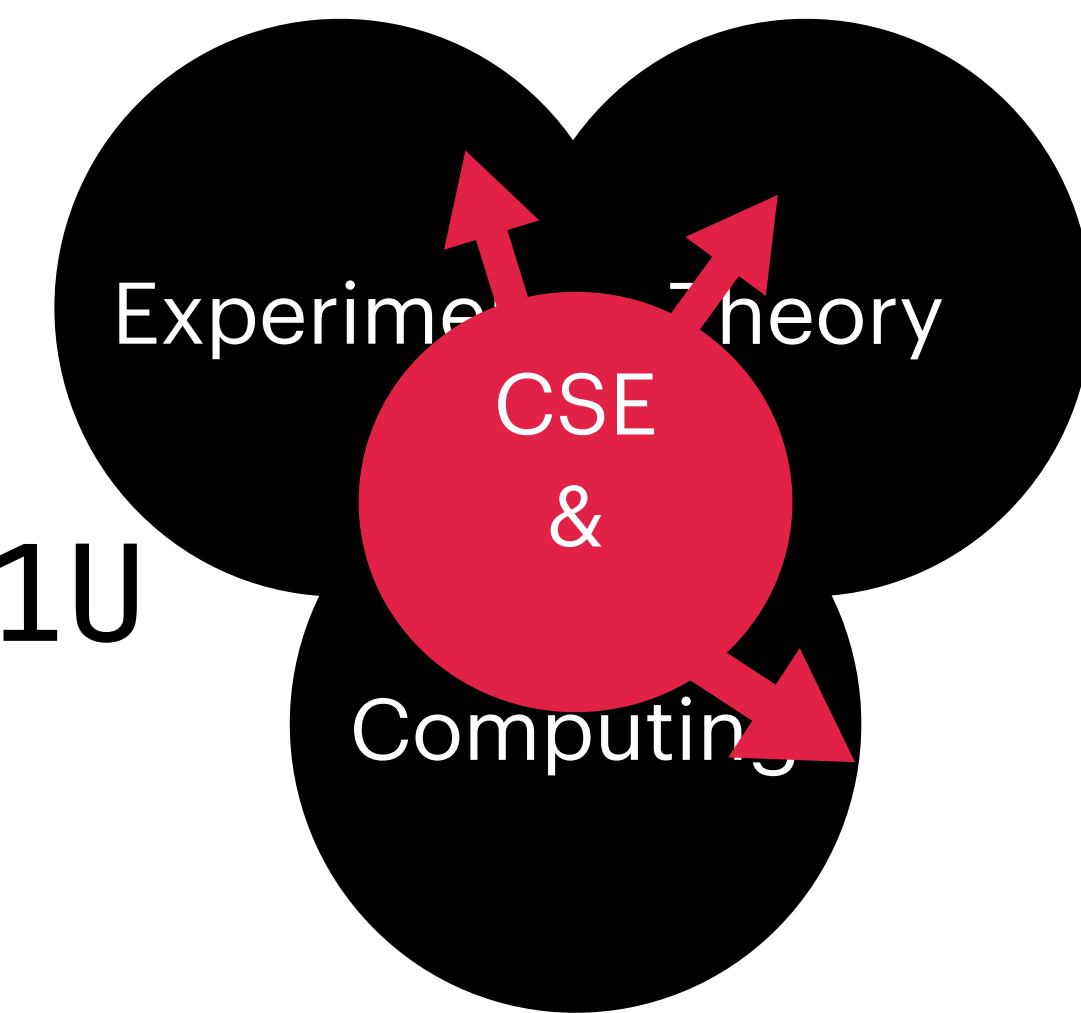
3V 1U

Quantum Information Processing I

Concepts and ideas of quantum information processing, quantum algorithms, quantum error correction, nature of quantum states and measurement.

(e.g. quantum circuits, gate decomposition and universal sets of gates, efficiency of quantum circuits, quantum algorithms (Shor, Grover, Deutsch-Josza,..), error correction, fault-tolerant design, entanglement, teleportation and dense coding, teleportation of gates, and cryptography)

2V 1U



Particle Accelerator Physics and Modeling I 2V 1U

Introducing particle accelerators from a theoretical point of view and covers state-of-the-art modelling techniques, we will develop a Python simulation tool.

(e.g. relativistic classical mechanics and electrodynamics, Lie algebraic structure of classical mechanics, linear symplectic maps, analysis of maps, symplectic particle tracking, collective Effects, linear & circular accelerators)

Particle Accelerator Physics and Modeling II 2V 1U

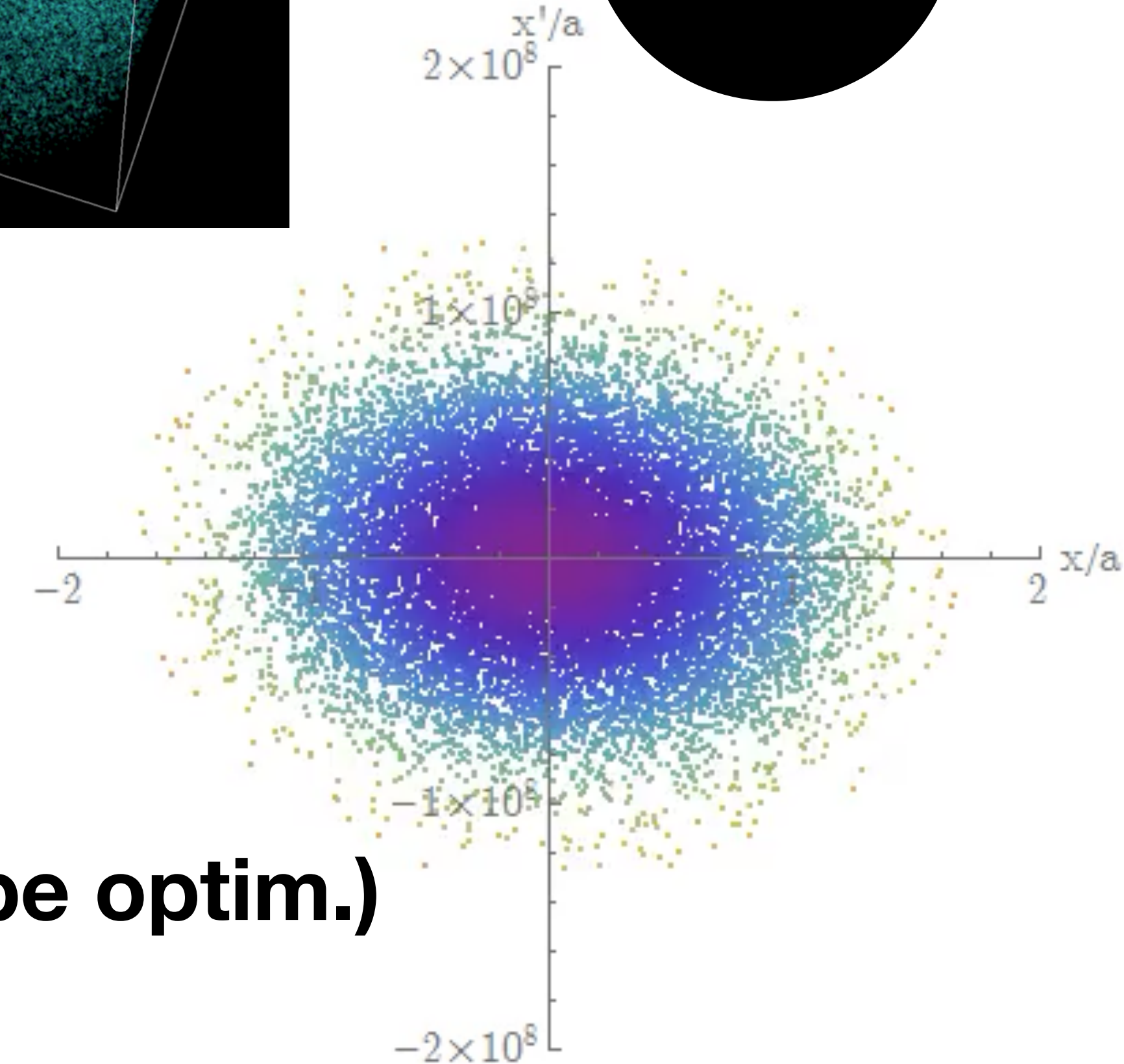
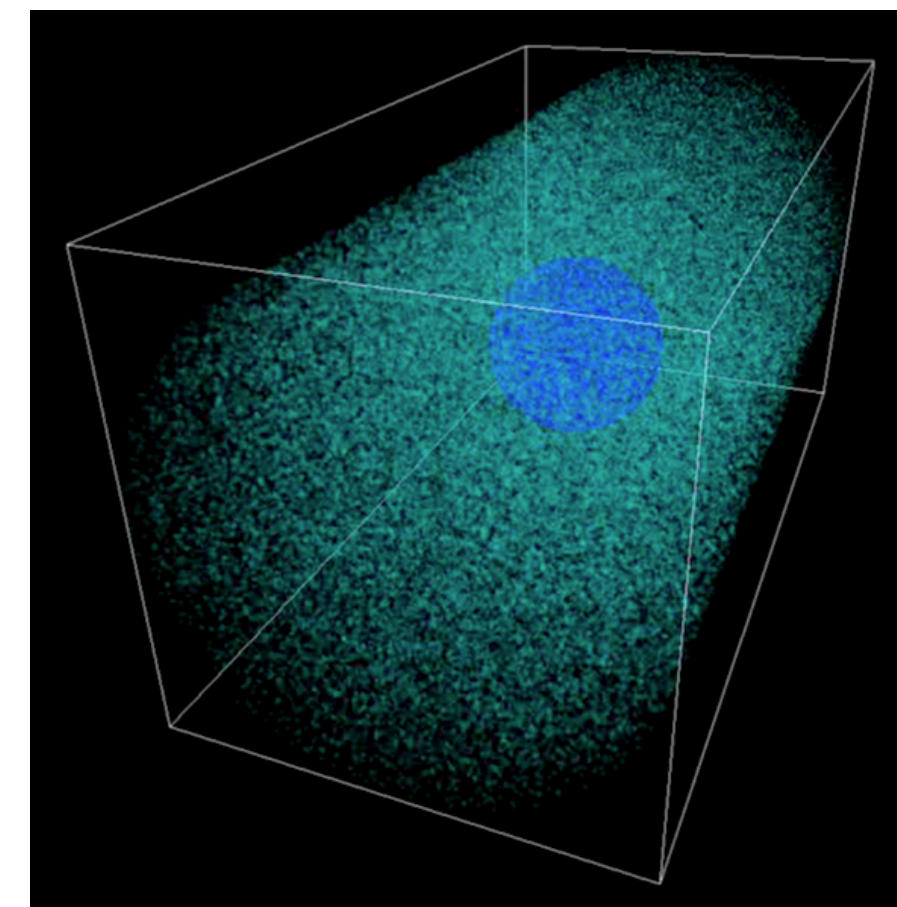
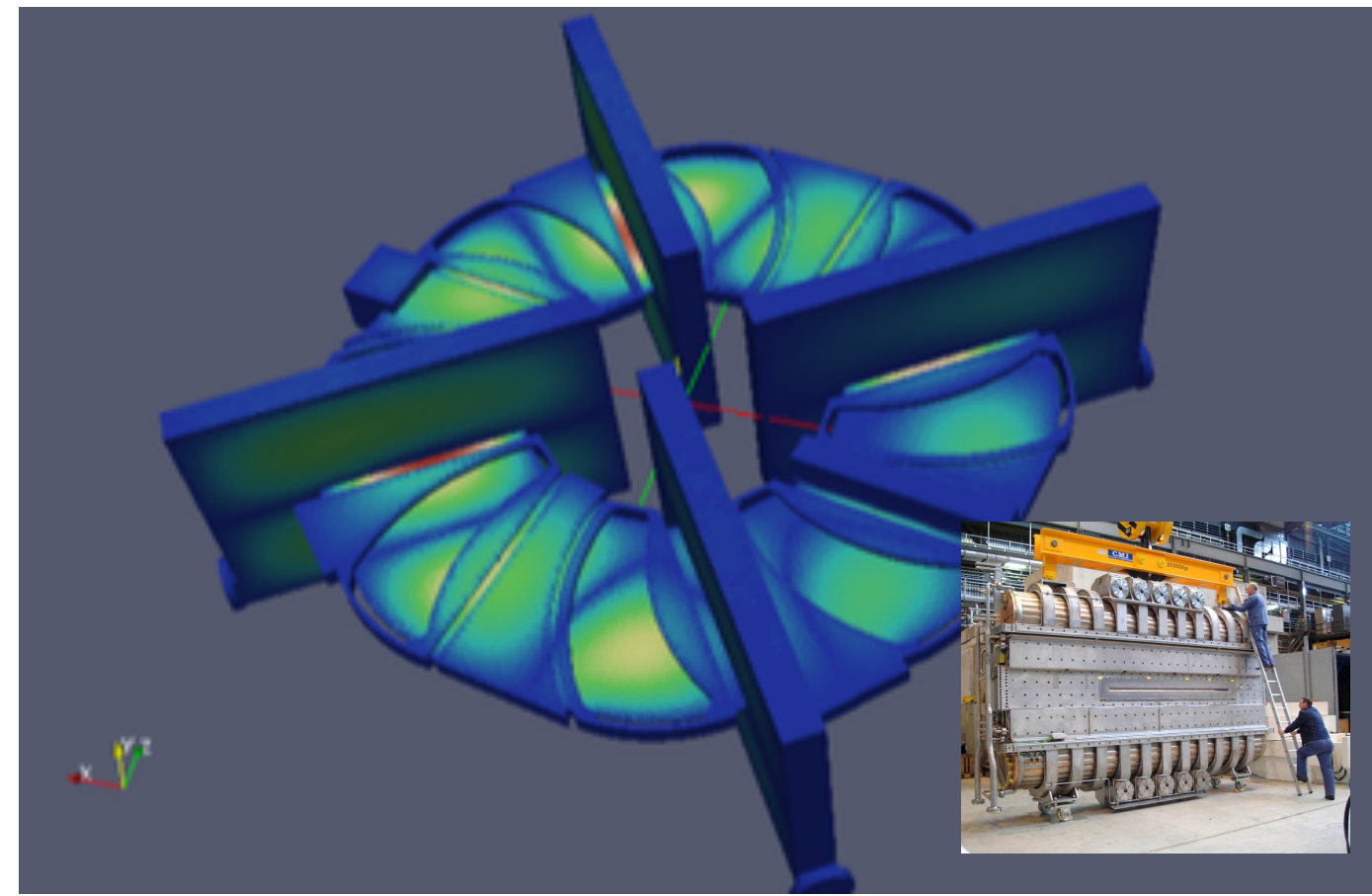
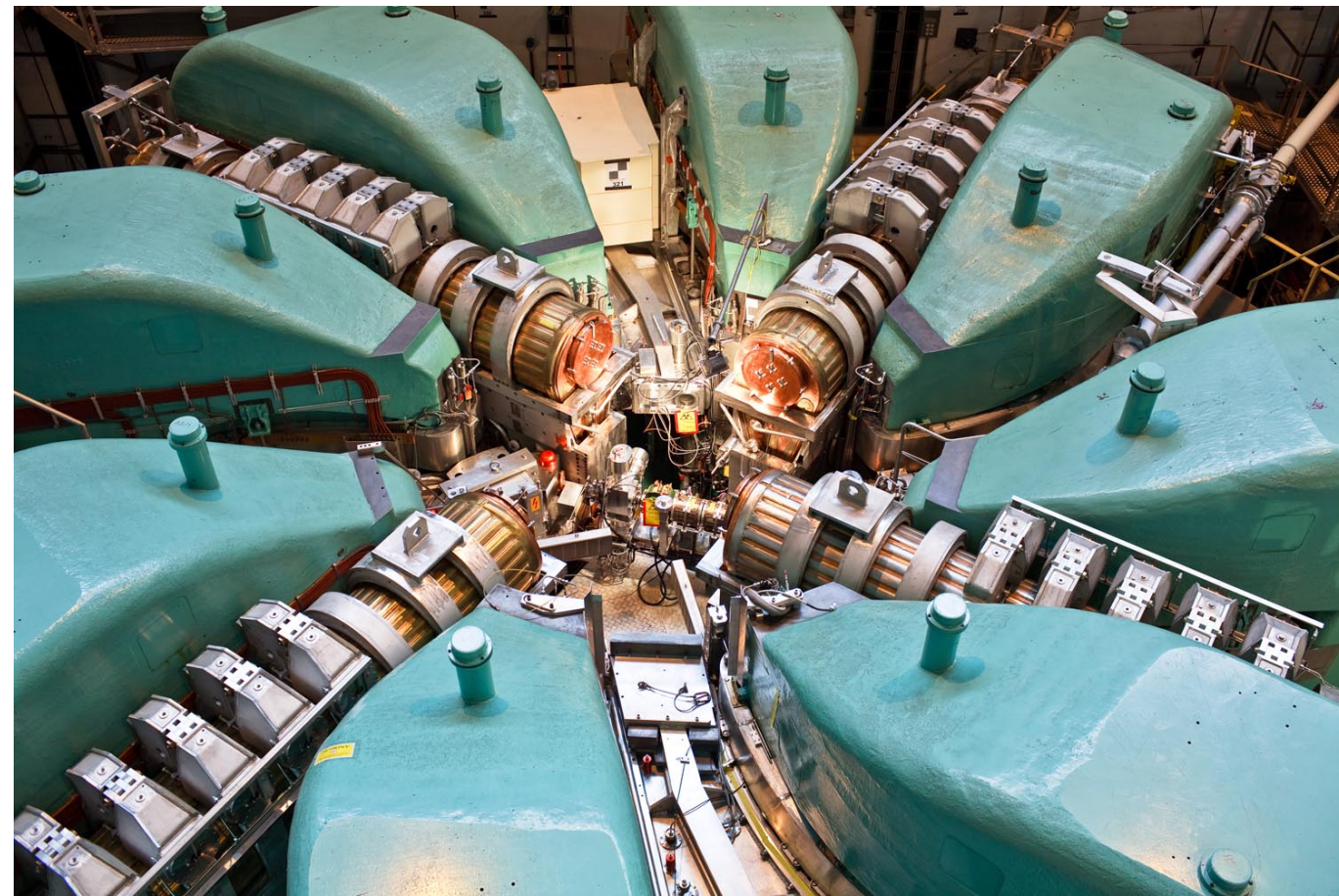
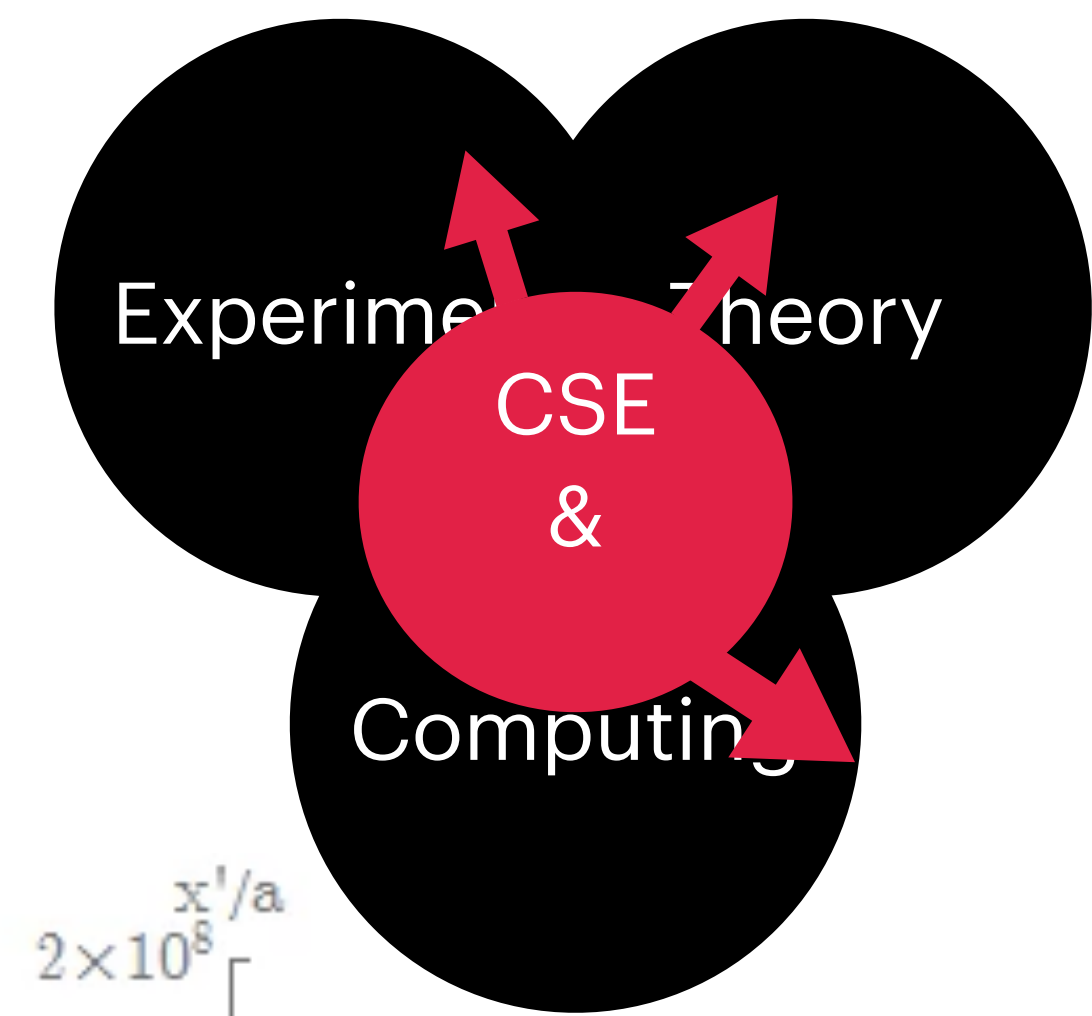
The accelerator will be viewed as a abstract dynamical system, effects of nonlinearities on the beam dynamics of charged particles will be discussed. Lie-Methods in combination with differential algebra (DA) and truncated power series (TPS) will be introduced. In the second part we will discuss surrogate model construction for such non-linear dynamical systems using neural networks and polynomial chaos expansion.

(e.g. symplectic maps and higher order beam dynamics, Taylor models and differential algebra, Lie methods, normal forms, surrogate models for dynamical systems, uncertainty quantification of dynamical systems)

Seminar in Physics for CSE RW 4

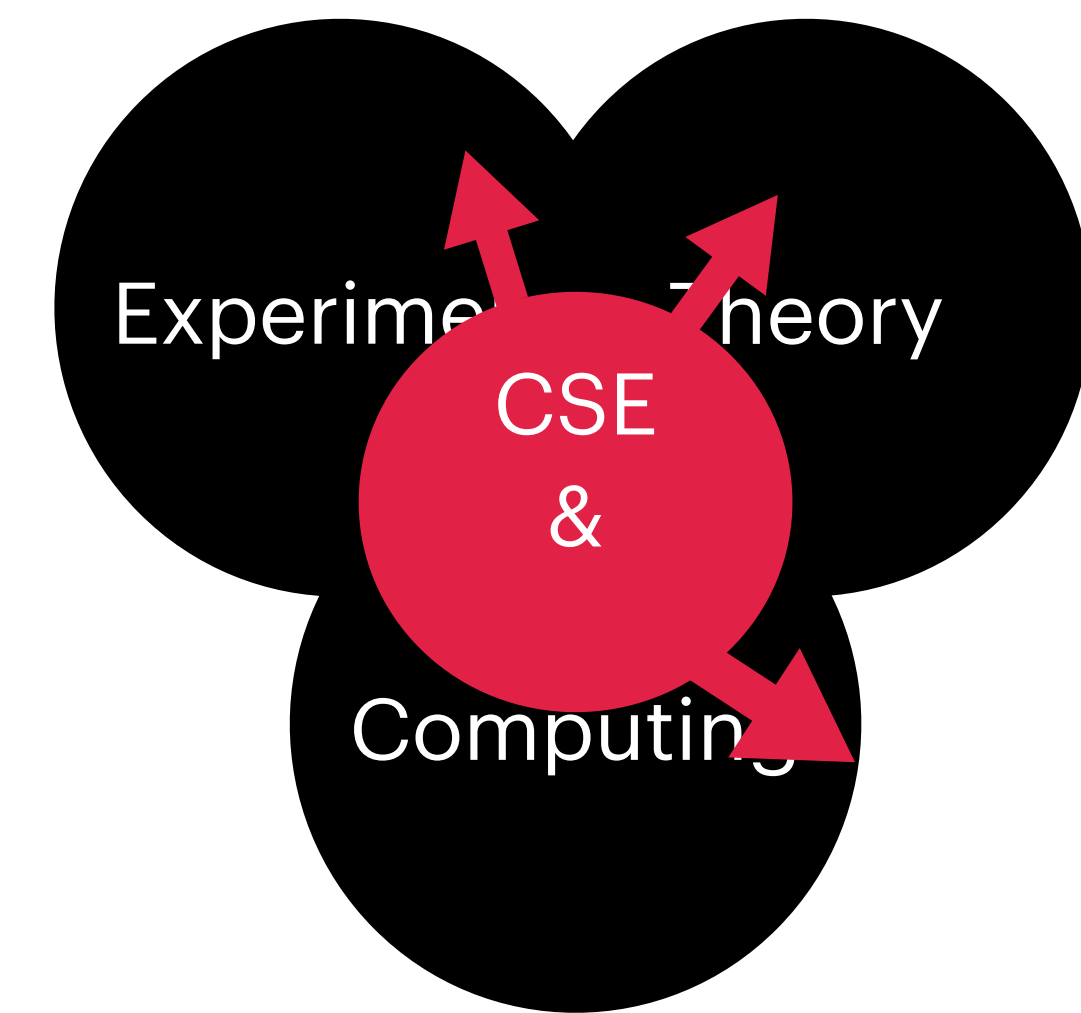
In this seminar the students present a talk on an advanced topic in modern theoretical or computational physics.

Accelerator Physics



- Solves 3D electric field vector wave equation
- FEM with unstructured tetrahedral mesh
- Model and optimise multiple objectives (GA, shape optim.)
- Largest scale commutation allows us to model largest structures

More Information



Vorlesungsverzeichnis

For question please contact me @ andreaad@ethz.ch

Seminar proposals: <http://amas.web.psi.ch/people/aadelmann/ETH-Accel-Lecture-1/seminar/>

Term and MSc projects: <http://amas.web.psi.ch/people/aadelmann/ETH-Accel-Lecture-1/projects/>

Completed projects: <http://amas.web.psi.ch/people/aadelmann/ETH-Accel-Lecture-1/projectscompleted/>