Ph.D course in Cognitive Neuroscience

Head of the Ph.D course: **Prof. Mathew Diamond**
Web site: **Cognitive Neuroscience**

Research project: **"High-throughput approaches to the study of rodent visual perception in behavioral neurophysiology experiments" in collaboration with CyNexo S.r.l.**
SISSA Supervisor: **Prof. Davide Zoccolan**
CyNexo è una start-up di ingegneria meccatronica applicata alla gestione della qualità, dei progetti e dei processi per istituzioni accademiche e private. Il team, nato all'interno della SISSA sviluppa hardware per laboratori scientifici, integrazione di sensori e software e lavora su piattaforme Industry 4.0 per supportare le piccole e medie imprese nell'adozione della giusta tecnologia per l'ottimizzazione della qualità e dei processi a ciclo chiuso.

CyNexo is a mechatronic engineering start-up applied to quality, project and process management for academic and private institutions. The team, born within SISSA, develops hardware for scientific laboratories, sensor and software integration and works on Industry 4.0 platforms to support small and medium-sized enterprises in adopting the right technology for the optimization of quality and closed-loop processes.

Research project: **"*Development of neuropsychological tools aimed at mapping the skills of persons with autism in corporate contexts*" in collaboration with CADIAI Coop. Sociale**
SISSA Supervisor: **Prof.ssa Raffaella Rumiati**
L'obiettivo principale del progetto è quello di sviluppare e validare strumenti per la valutazione e il monitoraggio di competenze utili all'inserimento e all'inclusione di persone con autismo in ambito aziendale. Tali strumenti riguarderanno la valutazione di competenze compito-specifiche (per es. competenze informatiche e digitali) e di dimensioni esecutive, trasversali e motivazionali nelle persone con disturbo dello spettro autistico. Inoltre, è prevista la registrazione di eventuali componenti dei potenziali evento-relati (ERP) che diano conto di differenze tra persone con autismo lungo le dimensioni sopra indicate.

The main objective of the project is to develop and validate tools for the evaluation and monitoring of skills useful for the insertion and inclusion of persons with autism in the corporate environment. These tools will concern the evaluation of task-specific skills (e.g. IT and digital skills) and executive, transversal and motivational dimensions in persons with autism spectrum disorder. Furthermore, the recording of any components of event-related potentials (ERPs) that account for differences between people with autism along the dimensions indicated above is envisaged.

Admission: **Academic and scientific qualifications + written test + oral exam**
Beginning of the Courses: **1 October, 2024**

Evaluation of academic and scientific qualifications: 10 points
Evaluation of Written Exam: 40 points
Evaluation of Oral Exam: 50 points

To be considered eligible, candidates must pass all the phases (academic qualifications, and interview) with a minimum mark of 7/10 or equivalent.
Results of all evaluations will be notified by email.

Deadline for online submission of applications: 27th August, 2024

Exams: **to be defined (beginning of September 2024)**

Ph.D course in Mathematical Analysis, Modelling, and Applications

Head of the Ph.D course: **Prof. Massimiliano Berti**
Web site: **Mathematical Analysis, Modelling, and Applications**

Research projects:

1. **"CFD enhanced solvers for advanced problems" in collaboration with Engys**
   Development of innovative methodologies enhanced by artificial intelligence and model order reduction for real time computing in computational fluid dynamics. The aim is an integration between HPC and model reduction, including uncertainty quantification, for complex simulation in presence also of turbulence patterns.

2. **"Real time computing and analytics enhanced by artificial intelligence and model order reduction" in collaboration with FAST Computing**
   Development of innovative methodologies enhanced by artificial intelligence and model order reduction for real time computing and analytics. The aim is an integration between data and models, HPC and model reduction, including uncertainty quantification.

3. **"Development of advanced reduced methods of parametric optimization for the structural analysis of cruise vessels" in collaboration with Fincantieri SpA**
   Development of integrated data driven tools governed by artificial intelligence for the hydrodynamic shape optimisation of innovative cruise ship vessels.

Admission: **Academic and scientific qualifications + oral exam**
Beginning of the Courses: **1 October, 2024**

Evaluation of academic and scientific qualifications: 30 points
Evaluation of Oral Exam: 70 points

To be considered eligible, candidates must pass all the phases (academic qualifications, and interview) with a minimum mark of 7/10 or equivalent.
Results of all evaluations will be notified by email.

Deadline for online submission of applications: 27 August, 2024

Oral Exam: 3-4 September, 2024

Ph.D course in Theory and Numerical Simulation on the Condensed Matter

Head of the Ph.D course: **Prof. Alessandro Silva**
Web site: [Theory and Numerical Simulation on the Condensed Matter]
Research projects:

"Compositional disorder and atomistic structure determination in computational materials discovery" in collaboration with Materys

Over the last decade, high-throughput ab initio simulations have been used to screen inorganic materials databases for target properties. However, computational materials screenings have typically targeted ordered crystalline compounds, leaving out materials with compositional disorder, such as solid solutions and alloys, which are abundant and technologically relevant. In addition, the usual experimental determination of the crystal structure through x-ray diffraction patterns might not be able to distinguish ordered from compositionally disordered crystals, hindering the sharp determination of the atomistic structure. In this project, we address the challenge of simulating compositional disorder in high-throughput mode. We will develop methods and software to automate ab initio simulations of crystal structures with fractional occupations and, in parallel, produce data-driven tools to determine accurate atomistic structures for compositionally disordered materials. Examples of potential foreseen applications include the discovery, design or optimization of metallic alloys (e.g., steel and superalloys) and candidate compounds for high-temperature superconductivity.

"Machine learning Wannier Hamiltonians for materials screening and large-scale electronic structure simulations" in collaboration with ENI

Wannier functions (WFs), and in particular maximally-localized Wannier functions (MLWFs), provide an accurate, compact, and localized representation of the electronic-structure problem, and have become widely used in computational condensed-matter physics and materials science. WFs can be obtained for isolated or extended systems (both crystalline and disordered), and can be used to understand chemical bonding, to characterize polarization, magnetization, and topology, or as an optimal basis set, providing very accurate interpolations in reciprocal space or large-scale Hamiltonians. In the last half of decade, the construction of WFs has been fully automated, but their applicability remains somewhat hindered by the computational cost of the underlying first-principles simulations.
In this PhD research project, we propose to develop machine-learning (ML) methods to calculate electronic Hamiltonians in the WF basis, and apply them to understand, discover and design novel materials. We will leverage automation tools that we have developed over the last years to construct first-principles training data sets at the level of density-functional theory or beyond, such as hybrid functionals or GW many-body perturbation theory. Millions of first-principles WF matrix elements will then be used to train dedicated ML model that will yield the electronic Hamiltonian and other operators for materials and molecular systems. The approach will enable accurate first-principles electronic structure simulations of large atomistic systems at low cost, with countless applications such as simulating the electronic structure of complex amorphous systems, finite-temperature simulations of optical properties, and fast screening of novel photovoltaics materials (e.g., perovskites), just to name a few.

Admission: Academic and scientific qualifications + oral exam
Beginning of the Courses: 1 October, 2024

Evaluation of academic and scientific qualifications: 30 points
Evaluation of Oral Exam: 70 points

To be considered eligible, candidates must pass all the phases (academic qualifications, and interview) with a minimum mark of 7/10 or equivalent.
Results of all evaluations will be notified by email.

Deadline for online submission of applications: 27 August, 2024

Oral Exam: to be defined - beginning of September 2024