



Leiden Institute of Advanced Computer Science (LIACS)

## “Smart Computing for Science & Industry”

### Introduction

LIACS is the Computer Science Institute of Leiden University, engaging in both research and education. We thrive on developing and improving methods, techniques and systems answering fundamental computer science questions and computer science solutions in life sciences, electronics, logistics, astronomic research, construction and engineering: **Smart Computing for Science & Industry.**

#### LIACS researchers engage in:

- **Data Mining and Decision Support**, with a focus on larger data volumes (“big data”) as well as on multi criteria decision support and optimisation.
- Design, implementation and application of **Advanced Computer Systems**, in particular parallel, distributed and embedded computer systems.
- Development of formalisms, methods, techniques and tools to design, analyse, and construct **Software Systems and Components**.
- Research on methods and techniques for the **Analysis and Synthesis of Images**, pattern recognition, 3D reconstruction and visualisation, image search and media technology.
- Transdisciplinary research into the relationships of **Information Technology Innovation** and social, organisational and business change.

### Mutual interest

Your organisation is at the forefront of your industry sector and is continuously looking for the next step. For example, in creating products that are more reliable, of higher quality, or more cost effective. Or you are looking for optimisation of the performance of production, transaction, analysis or innovation processes.

As an academic institute LIACS has a strong and vibrant research program in computer science with a good balance of core computer science and practical applications. Its strong research programs make LIACS also an attractive place for education. It takes care of the Bachelor Program Informatics (BSc) and Master Programs (MSc) on Computer Science, ICT in Business and Media Technology.

At LIACS we are interested in bringing our academic results into the marketplace, either as a service to industry, by joint research, by offering expert advice, as a playground for students or as employment for our graduates.

## What we can bring to the table

In order to facilitate the transition from computer science research into workable applications, we have defined a number of discrete services to offer you. Please contact us to discuss these opportunities and associated terms.

- **Custom solution development** where we work for your organisation to develop a solution, either as a consulting project with a report about our findings, or even developing a custom software solution to your task at hand.
- **Joint research projects** where we work together usually for a longer period of time with your organisation, whereby we both bring our specific expertise into the project to realise common objectives. For these projects we have a strong preference for academic research, i.e. supported by funding from EU, NWO, STW, etc.
- **Creative think-tank sessions** are used both as an education tool for students as well as a solution development session for your organisation. It requires thorough preparation and can be used to generate new applications, new services, new benefits, new strategies, etc. As a side effect the results may be used as input for further research or a master thesis project.
- **Master thesis internships** serve as a means for students to materialise their research into a coherent academic report. The subjects for internships can vary along the entire discipline portfolio of LIACS, but also multidisciplinary projects on the outer limits of the portfolio are very welcome.
- Researchers at LIACS are most of the time engaged in publicly funded projects, during which PhD's are working for 3- 4 years on fundamental scientific subjects. The results developed during the research program are made available as **Technology Offers**. This can be a method, an algorithm, a software tool, a prototype model, etc.
- As an acknowledged research institute LIACS has a high level of computer science expertise available. With **Expert Advice** we can help you to solve your computer science challenges, with which you can become more competitive in your marketplace.
- Every year about 40 master students graduate at LIACS and 10-15 PhDs receive their doctorates. Their specific expertise is highly appreciated by businesses, NGO's and governments. We know that identifying, selecting and hiring a new employee is a costly process. We can help you finding the **best recruits** for your organisation.

## Computer Science Community

Our drive is to make our science smart enough to make a lasting difference in society. Research at LIACS therefore has a clear relationship with day-to-day business challenges. In order to develop and maintain these relationships we are building a Computer Science Community of companies, NGO's, students and staff.

The anticipated benefit of this community is to have a two-way platform of interaction where thoughts develop into concepts, which develop into projects, which develop into solutions. If you want to be part of this community to bring and get insights you need, do not hesitate to contact us.

## Existing Collaborations

We have a strong focus on providing “Smart Computing for Science & Industry”. This focus materialises in our longstanding collaborations with industrial partners and governments. These collaborations help us to focus on the applicability of research results and at the same time it generates new directions for our research in computer science.

Our collaborations include partners such as BMW, Shell, Achmea, Honda, Tata Steel, Ministry of Water & Transport, Volker Infra, ProRail, KPMG, KPN, GE, Zorginstituut, Politie, DNB, etc.

## Contact

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# A diverse selection of projects at LIACS

## [Process mining for multi-objective online control](#)

In order to optimize the production and forming process of steel coils, PROMIMOOC aims at developing a generic platform to collect and integrate the data from the production process, model the process based the data, perform multiple-objective decision making based on data-driven models and finally give Pareto-optimal process control settings under complex constraints.

## [Annotated Graph Mining: finding a new balance between analysis of the graph structure](#)

This VIDI project aims at developing a new paradigm for data mining, one that is based on the analysis of annotated graphs. These are graphs where nodes and edges are annotated with extra information. The analysis of such graphs comprises both analysis of the graph structure and of the annotations. With this novel representation, data mining methods can be developed that strike an ideal balance between analysis of the graph structure, and analysis of the information in the annotations, and thus combine the advantages of the different approaches to relational mining that currently exist.

## [InfraWatch: monitoring and large-scale modeling of sensory data](#)

This recently started project is concerned with the monitoring and large-scale modeling of sensory data collected at the Dutch highway bridge "Hollandse Brug". 145 sensors plus a weather station and video camera produce a continuous stream of data under different traffic and weather situations. Our goal is to use this data to model the structural characteristics of the bridge over a long period.

## [CATCH LINKS: a multidisciplinary collaboration of computer science and history.](#)

In the early 1800's, municipalities in the Netherlands started to systematically record key population events, such as births, marriages and deaths. Recently, these data have been digitized to a considerable degree. Without unique identifiers, reconstructing relations in this data becomes a research problem. Besides relation discovery (known as 'record linkage'), also domain knowledge discovery and visualization are interesting from a data mining point of view.

## [CORTANA: A Data Mining tool for discovering local patterns in data.](#)

Cortana features a generic Subgroup Discovery algorithm that can be configured in many ways, in order to implement various forms of local pattern discovery. The tool can deal with a range of data types, both for the input attributes as well as the target attributes, including nominal, numeric and binary.

A unique feature of Cortana is its ability to deal with a range of Subgroup Discovery settings, determined by the type and number of target attributes. Where regular SD algorithms only consider a single target attribute, nominal or sometimes numeric, Cortana is able to deal with targets consisting of multiple attributes, in a setting called Exceptional Model Mining.

## [EvoMPP: designing femtosecond laser pulses to control atomic and \(bio\)-molecular dynamics.](#)

The motivation for this project was the realization that systematic trial-and-error-based variations of all parameters is often not possible in a many-parameter physical system. Consequently, it was proposed to study this class of problems by a new approach based on evolutionary algorithms (closed loop optimization). This project forms a bridge between researchers in mathematics, computer science and physics and aims to make new evolutionary approaches available to physics research involving large numbers of parameters, where traditional physics methodologies fail. Special focus is placed on the design of shaped femtosecond laser pulses to control atomic and (bio)-molecular dynamics and the control of DNA functionality in biological cells.

## [DELIVER: Distributed Coordination for Continuous Planning](#)

The DELIVER project aims to develop a novel approach towards logistic planning is developed, called continuous planning, as opposed to traditional (batch-oriented, a priori) planning.

The participation of many industrial partners in the project underlines the technical innovation of the project - the continuous planning approach is seen by many as a promising way to complement traditional planning

methods, in particular for planning on the day-of-delivery. The interest from industry shows that the project results will have a strong economical impact if proven successful.

#### **RODEO: Robust Design Optimization**

The RODEO project aims to find solutions that are optimal with respect to performance in the theoretical optimization model, but also good/stable with respect to variations caused by uncertainties or noise. Robust optimization is therefore aimed at finding optimal solutions that are also meaningful in practice.

Two practical optimization problems are studied as test-cases within this research are 1) automated design of drug molecules 2) robust design of a draw bead process.

In the automated design of drug molecules the assessment of the quality of candidate solutions is vaguely defined and methods are needed to still provide promising solutions, despite the uncertainty in the quality assessment. In the robust design of a draw bead process the aim is to design a process that yields proper parts, but which requires minimal material. Here it is very important to find solutions that are also stable variations of the material properties.

#### **BuildEnergyOpt: Energy and Thermal Comfort Optimization in Building Performance Design**

It is estimated that heating and cooling systems of buildings nowadays are a major part of the overall energy consumption (ca. 30%). To reduce this consumption, modifications of build environments are needed, ideally without deteriorating other performance criteria, such as thermal comfort and health. To contribute to this multi-objective design task we develop multi objective optimization algorithms based on building performance simulation.

Building performance simulation (BPS) is a powerful tool to predict and analyse the dynamic behaviour of indicators such as energy consumption and thermal comfort in building. In this project we hypothesize that introducing a design optimization capability to BPS tools can provide valuable support in decision making. Advanced algorithms for multi-objective optimization are assessed for their future integration in building performance tools.

#### **Project LigOpt: Multi-objective ligand design**

The protein family 14-3-3 is involved in many signalling networks of the human body. It has different isoforms, some of which are involved in life maintaining functions, others (the gamma isoforms) are part of processes related to Alzheimer and cancer. Therefore it is desirable to find a molecule that specifically binds to gamma isoforms but not to the other isoforms of 14-3-3.

Peptides are sequences of amino-acids - each amino acid is taken from an 'alphabet' of 18 possibilities. To find optimal sequences force field simulation (evaluation) is combined with multi objective combinatorial black-box optimization. For short sequences deterministic procedure ILS is used and extended sequences are searched for by multi objective evolutionary algorithms.

#### **3D Imaging of development in Zebra fish**

The zebra fish is an important model system in developmental genetics and biology. 3D imaging offers us challenges in the manipulation of large numbers of 3D data as well as the integration of different types of 3D microscopy data, i.e. images. Upon its introduction in life science research a swarm of information is produced. Amongst others (ZFIN) we are involved in finding solutions and new approaches in the processing of the data generated by zebra fish research. Integration of these data with other resources is crucial. Following the original work in the 3D atlas of zebra fish development several new projects have started in recent years.

We work with Confocal and Multi Photon Microscopy, serial sections (atlas) and Magnetic Resonance Microscopy (MRM).