

# COMPUTATIONAL SCIENCE AND ENGINEERING (CSE)

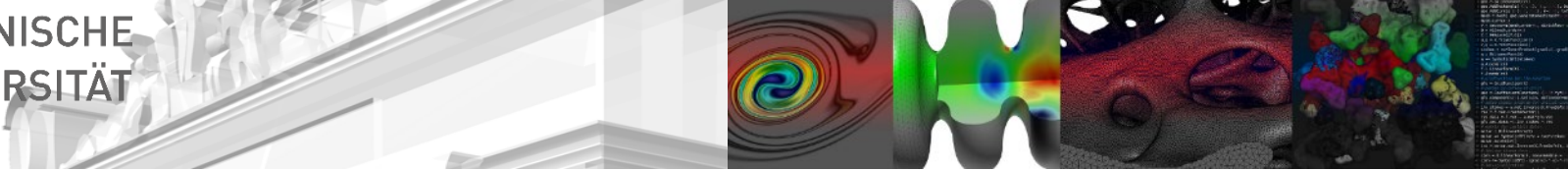


*Interdisciplinary Master's Program in English*

*[tuwien.at/cse](http://tuwien.at/cse)*

*[cse-master@tuwien.ac.at](mailto:cse-master@tuwien.ac.at)*

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**Institute of Materials Chemistry**



## The goals of computational materials science

New technologies require very specific functionality. E.g.:

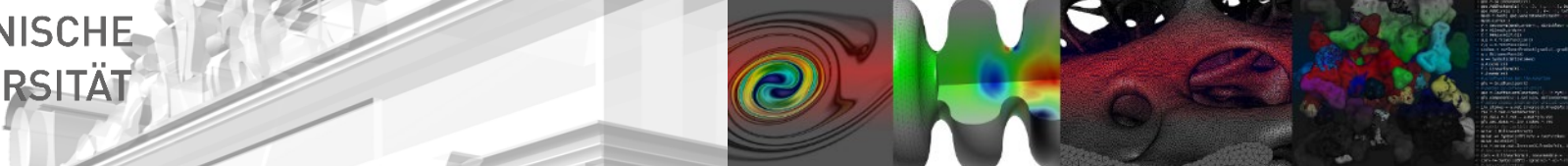
- More efficient solar cells
- Energetically denser, longer-lasting batteries
- Lighter structural materials
- Hard magnets without rare earths

Often:

- Functionality well understood
- Materials unknown (if they even exist)

Basic question:

**Which materials offer specific features X, Y and Z under conditions P and Q?**



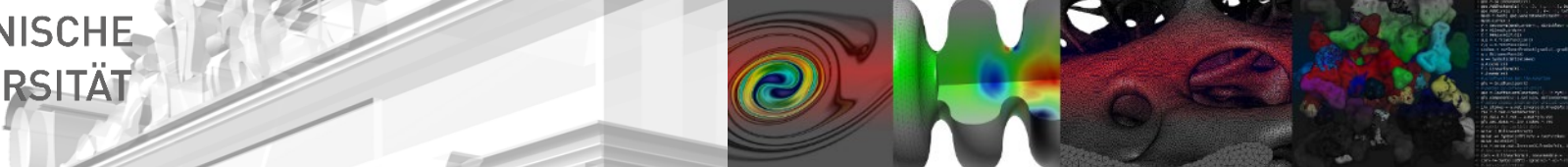
## What about computational chemistry?

Parallel problem. Societal problems demand compounds with specific functionality. E.g.:

- More efficient catalysts
- Better lubricants
- More stable battery electrolytes
- New antivirals and other pharmaceuticals
- Very specific solvents

Basic questions:

**Which compounds (and processes) offer properties X, Y and Z under conditions P and Q?**



## An ongoing paradigm change

### Old computational chemistry and materials science

- Analysis of known materials/compounds
- Qualitative results
- Plenty of experimental input
- Constant human intervention

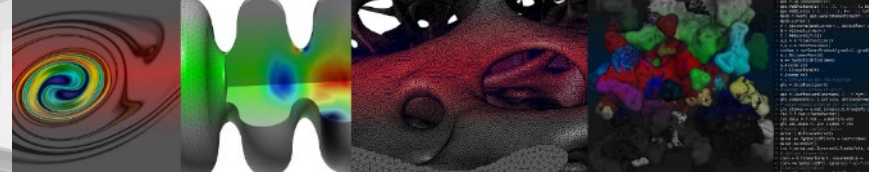
### New computational chemistry and materials science

- Ab-initio
- Quantitative results
- Speculative materials/compounds
- High throughput
- Inverse design

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### This change has analogues in most areas of science and engineering

- Propelled by advances in hardware and algorithms
- Connected to the big data revolution



# An emerging area: Computational Science and Engineering

In short: How to **efficiently use** these ...



```
#include <iostream>
#include <omp.h>
main(int argc, char *argv[])
{
    int i;
    int N = 1000;
    int chunk = 100;
    std::vector<float> a(N), b(N), c(N);
    /* Some initializations */
    for (i=0; i < N; i++)
        a[i] = b[i] = i * 1.0;
    #pragma omp parallel shared(a,b,c,chunk) \
        private(i)
    {
        #pragma omp for
        for (i=0; i < N; i++)
            c[i] = a[i] + b[i];
    } /* end of parallel region */
}
```

$$H\psi = E\psi$$

$$\nabla^2 u = \nabla \cdot \nabla u = f$$

$$m\ddot{r} = f$$

... to **simulate cutting-edge problems?**

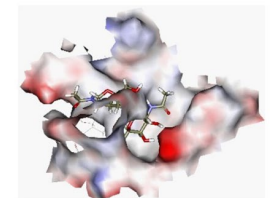
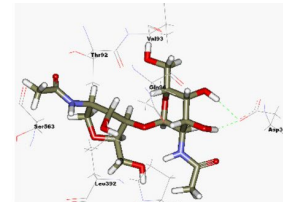
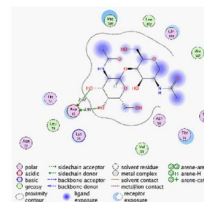
For instance, how to simulate the binding of molecules to a COVID-19 virion?

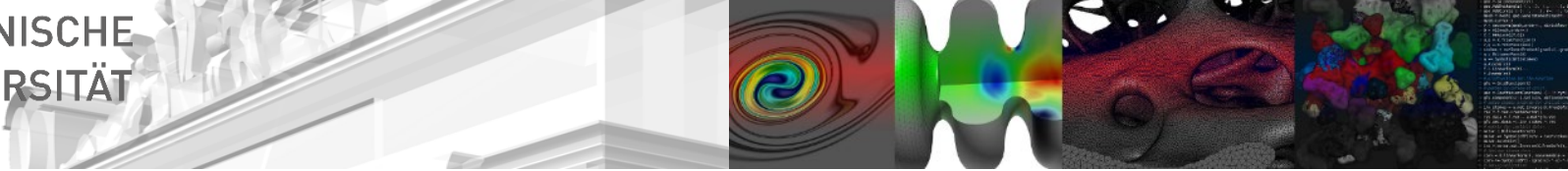
ORIGINAL RESEARCH  
published: 04 May 2021  
doi: 10.3389/fchem.2021.661230



## Molecular Docking and Dynamics Simulation Revealed the Potential Inhibitory Activity of ACEIs Against SARS-CoV-2 Targeting the hACE2 Receptor

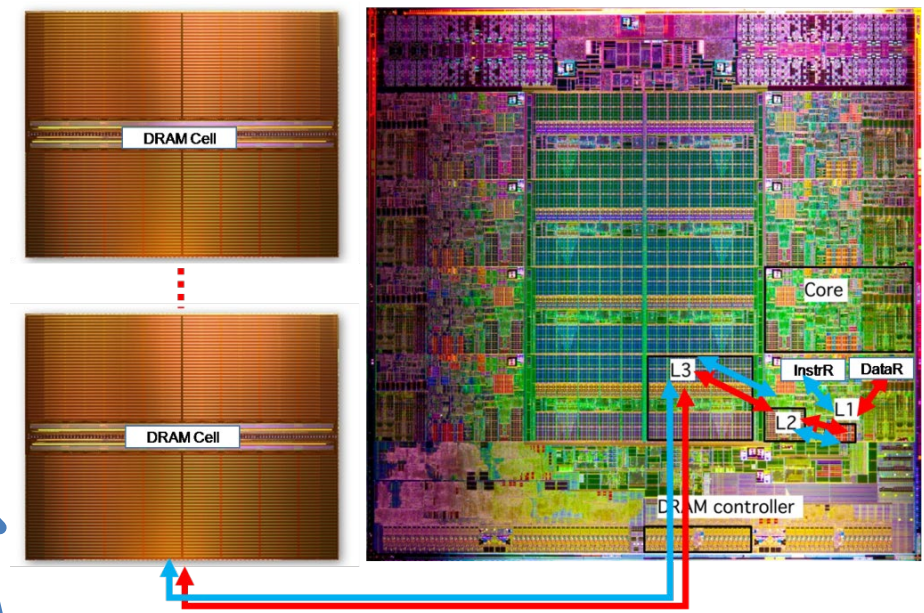
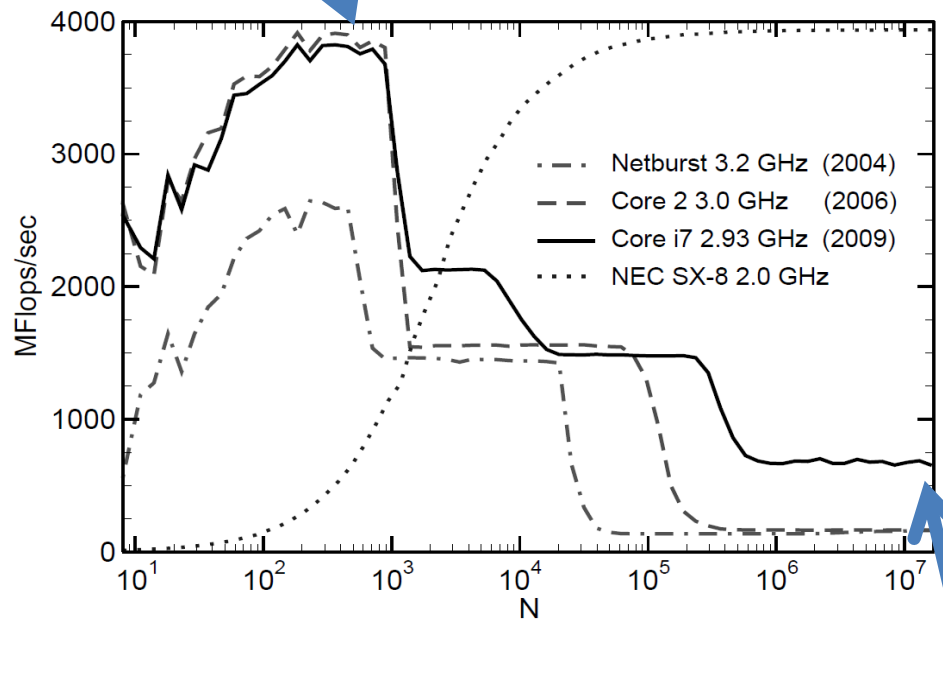
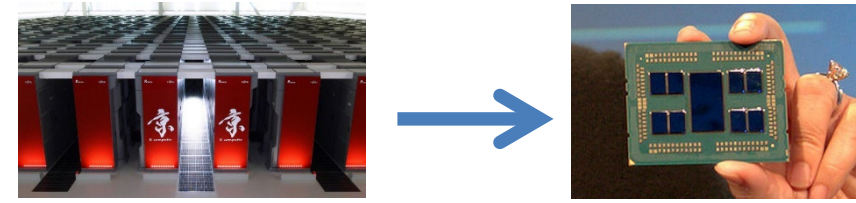
Ahmed A. Al-Karmalawy<sup>1</sup>, Mohammed A. Dahab<sup>2\*</sup>, Ahmed M. Metwally<sup>1</sup>, Sameh S. Elhady<sup>1</sup>, Eslam B. Elkaeed<sup>3,4</sup>, Ibrahim H. Eissa<sup>2\*</sup> and Khaled M. Darwish<sup>1</sup>



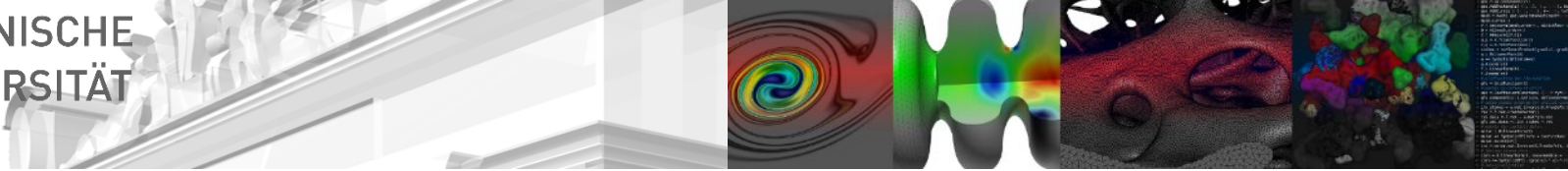


# What is Computational Science and Engineering?

## Peak performance?



## Max. bandwidth?



## What is Computational Science and Engineering?

Or, to put it in words ...

### IEEE:

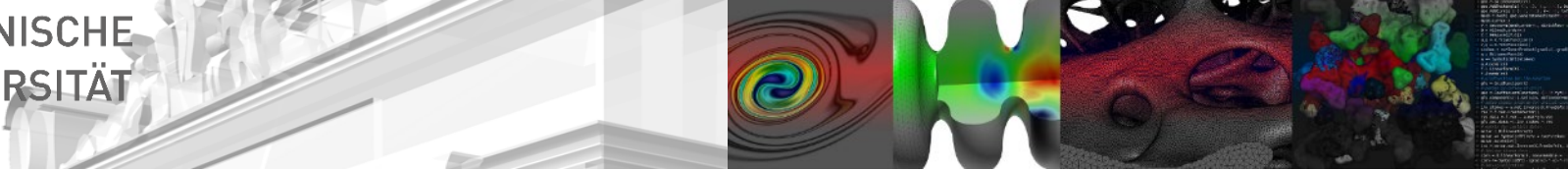
*... science (and engineering) that is "computational" as opposed to "experimental" or "theoretical"*

### Krell Institute:

*... computational science involves using computers to study scientific problems and complements the areas of theory and experimentation in traditional scientific investigation.*

### SIAM:

*CSE focuses on the development of problem-solving methodologies and robust tools for the solution of scientific and engineering problems. We believe that CSE will play an important if not dominating role for the future of the scientific discovery process and engineering design.*



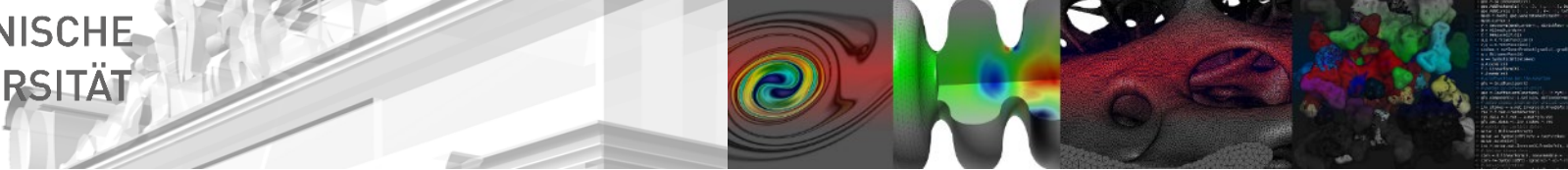
## Is the Computational Science and Engineering Program for You?

Are you interested in

- ... implementing efficient computer programs?
- ... solving mathematical problems with the computer?
- ... modeling arbitrary physical processes?
- ... utilizing supercomputers?
- ... a program in English with an international vocation?

If you reply to most of these questions with *“yes”*, then you have your answer.

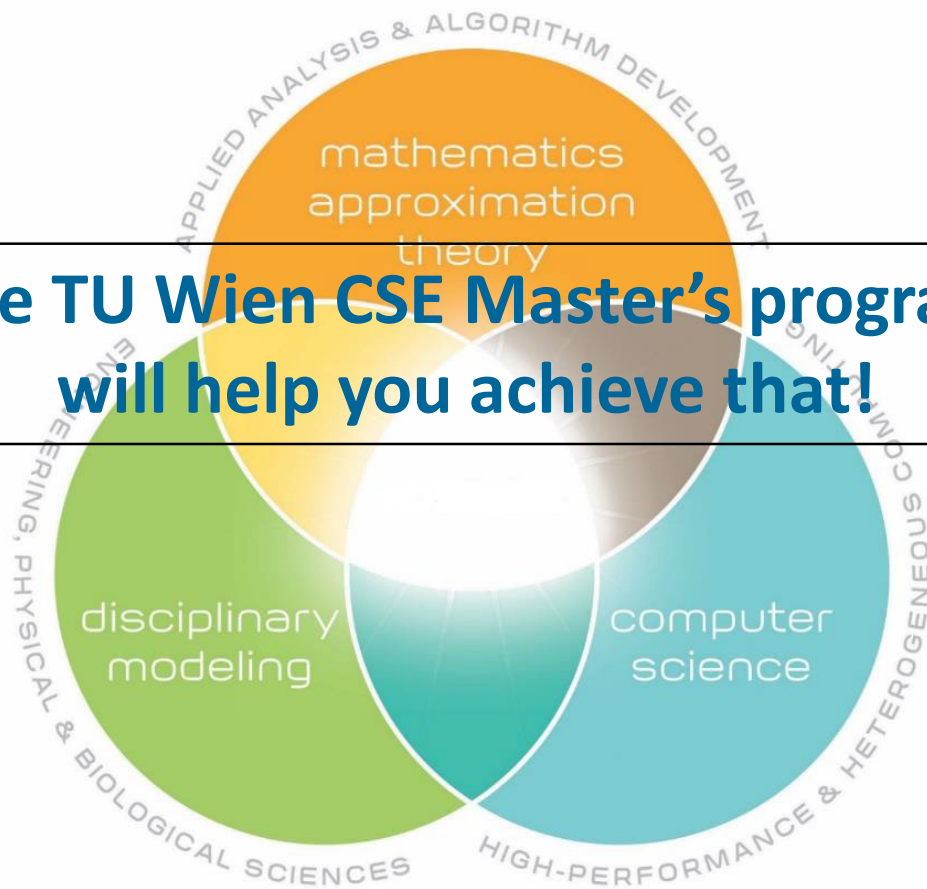


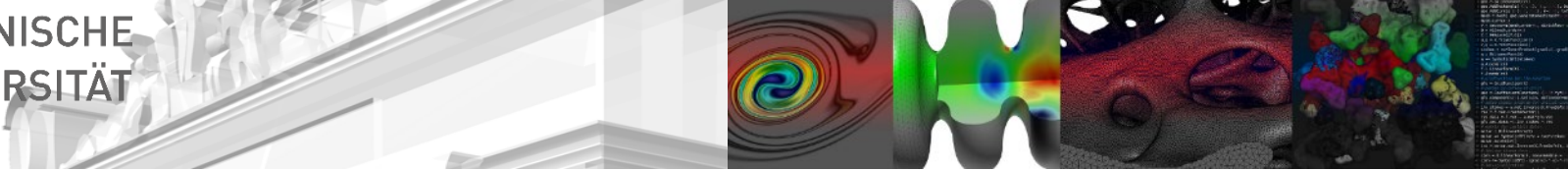


## What is Needed to Become Successful in CSE?

You need to get proficient in three main areas:

**The TU Wien CSE Master's program  
will help you achieve that!**

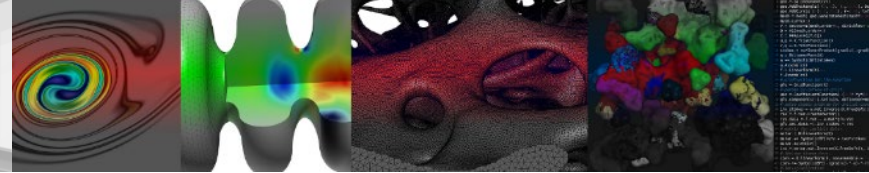




## Where is CSE Applied?

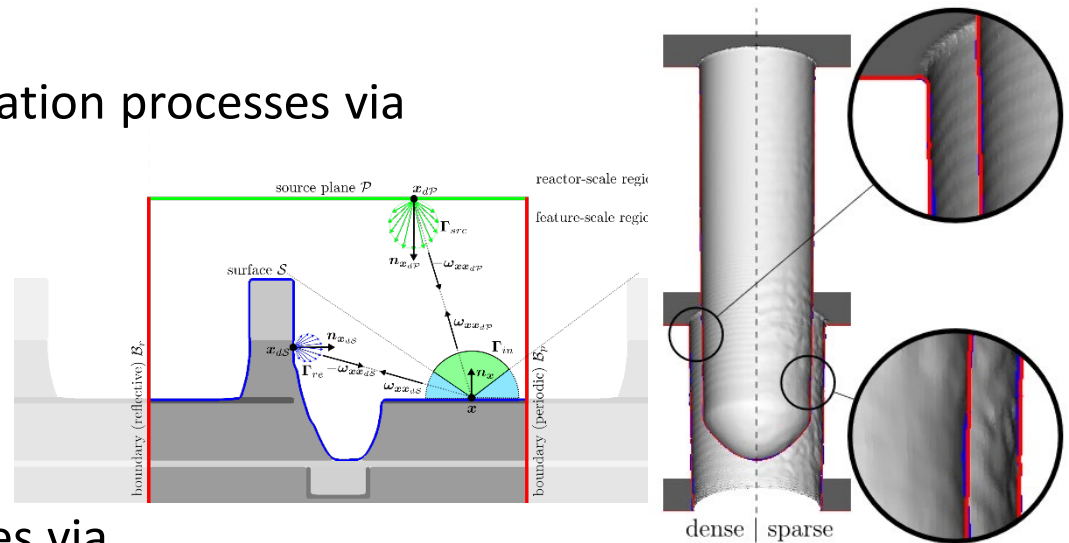
- Electronics
- Chemistry & Materials Science
- Building Science
- Mathematics
- Fluid Dynamics & Acoustics
- Informatics
- Solid Mechanics
- Mechatronics
- Finance
- Medicine
- etc.

*\*) Blue application areas can be studied as part of selectable key areas in the TU Wien CSE Master's program.*

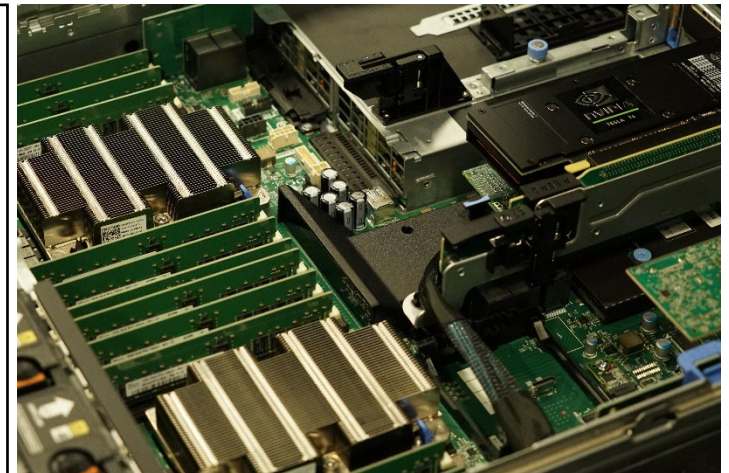
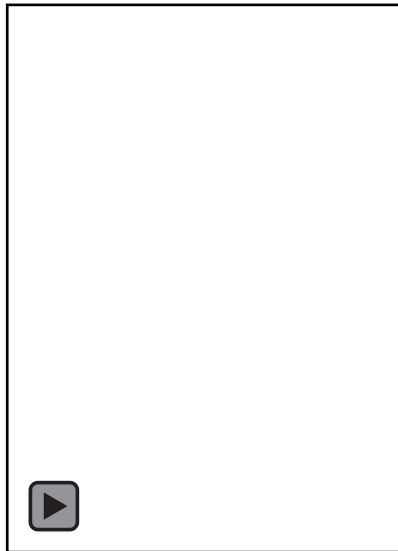


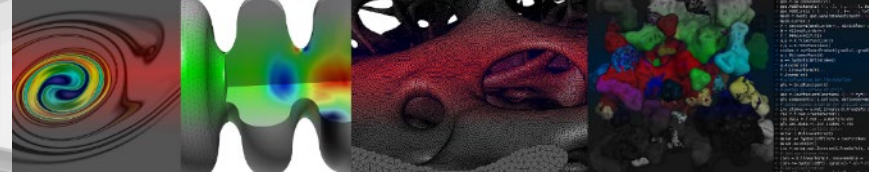
# Computational Electronics

- Simulate semiconductor fabrication processes via
  - level-set solvers
  - ray-tracing methods
  - machine learning tools
  
- Simulate semiconductor devices via



- Monte Carlo solvers
- finite difference/  
volume/  
element solvers

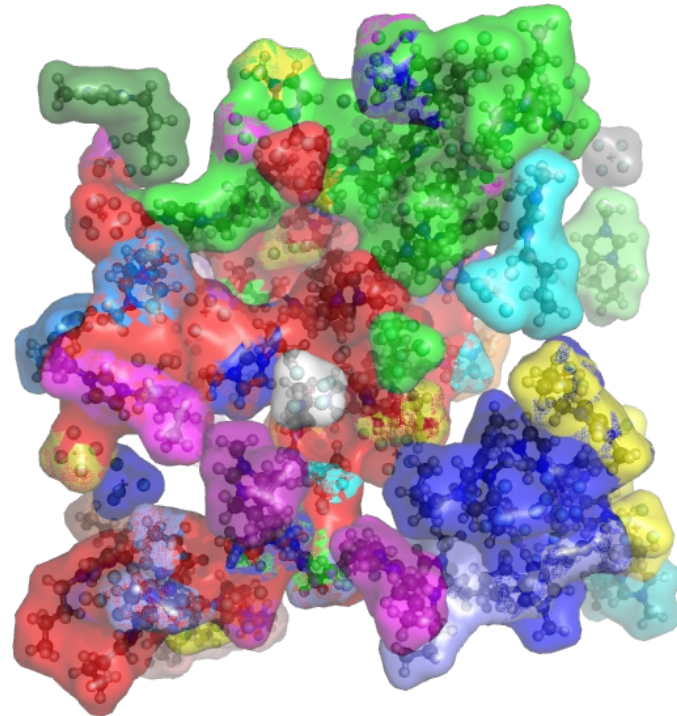
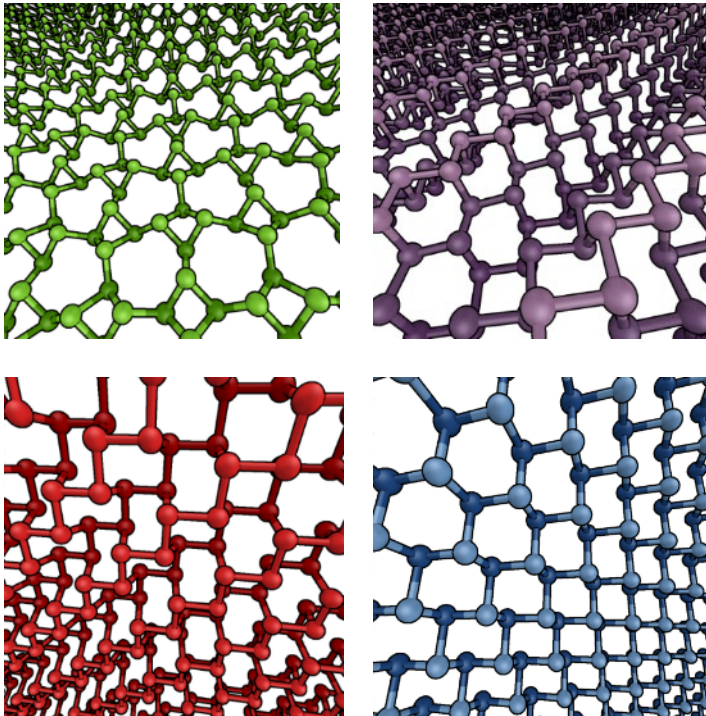


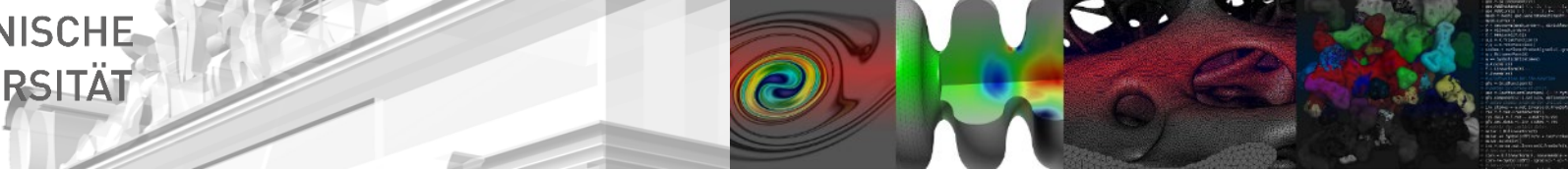


## Other Key Areas at TU Wien

### Computational Chemistry & Materials Science

*... simulate atoms and molecules*

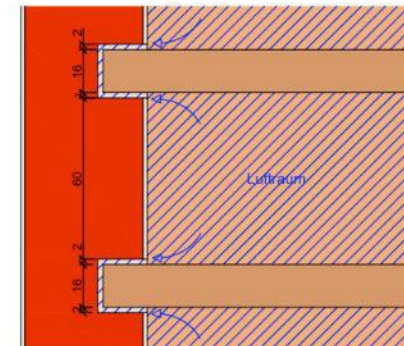
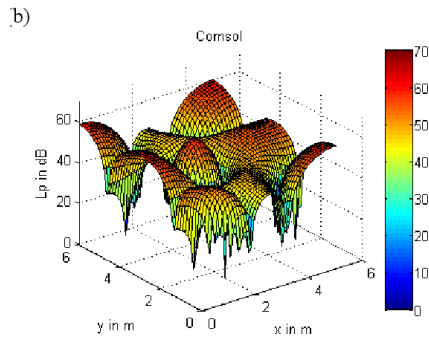
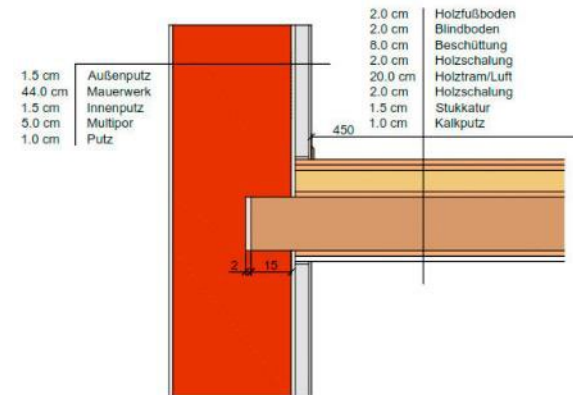
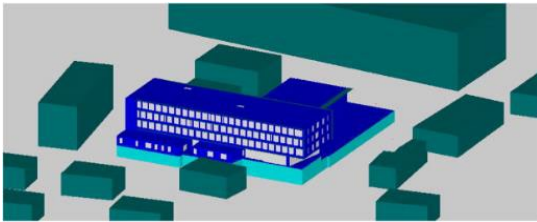




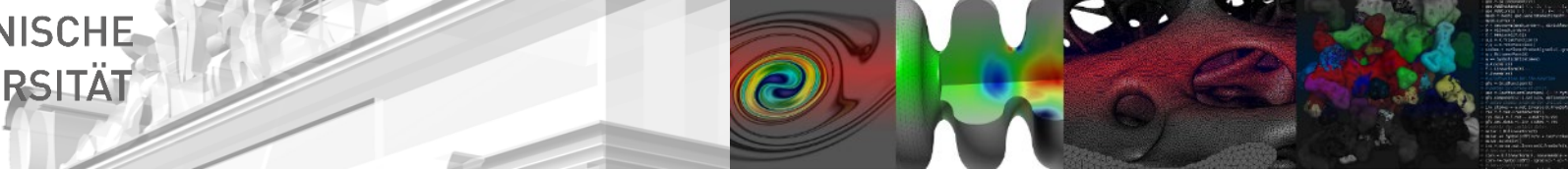
## Other Key Areas at TU Wien

### Computational Building Science

*... simulate buildings*



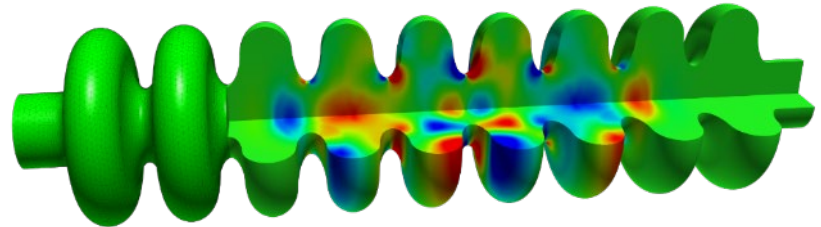
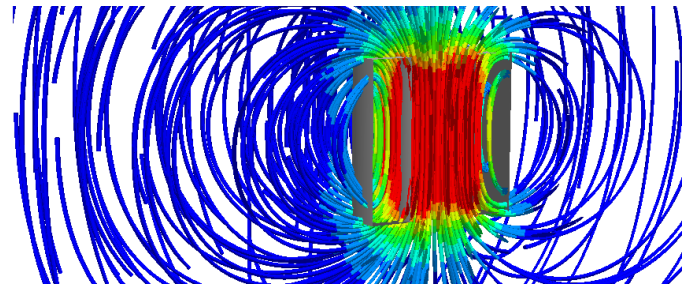
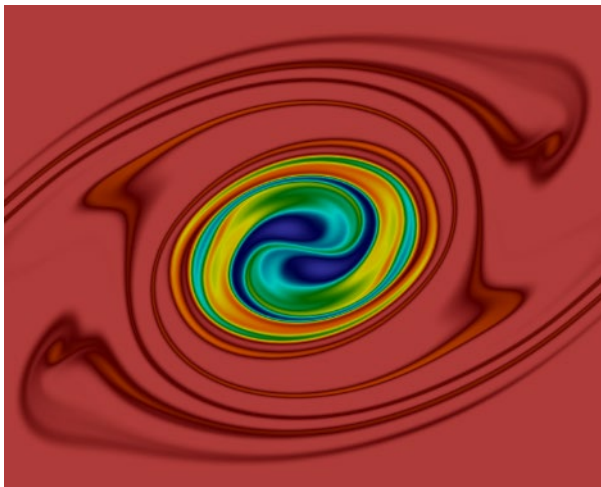
Source: Wegerer, Bednar, Energy Procedia, 2017



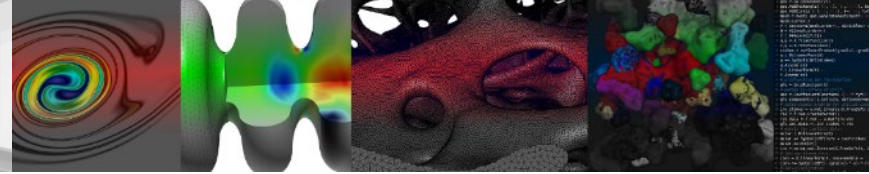
## Other Key Areas at TU Wien

### Computational Mathematics

*... simulate particularly challenging problems*



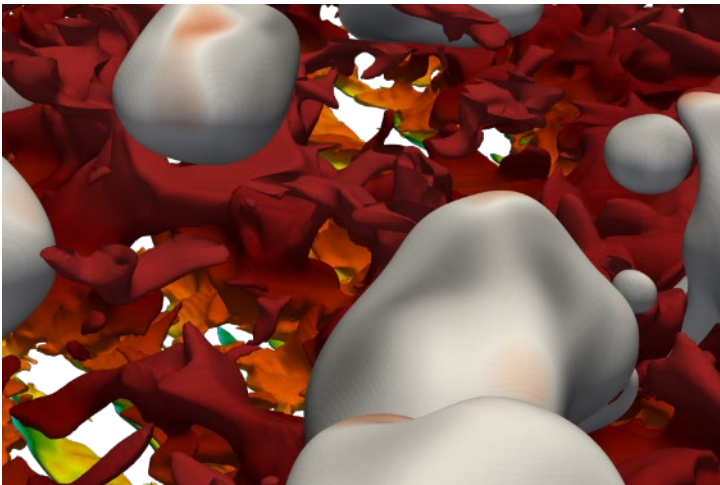
Source: Schöberl, TU Wien



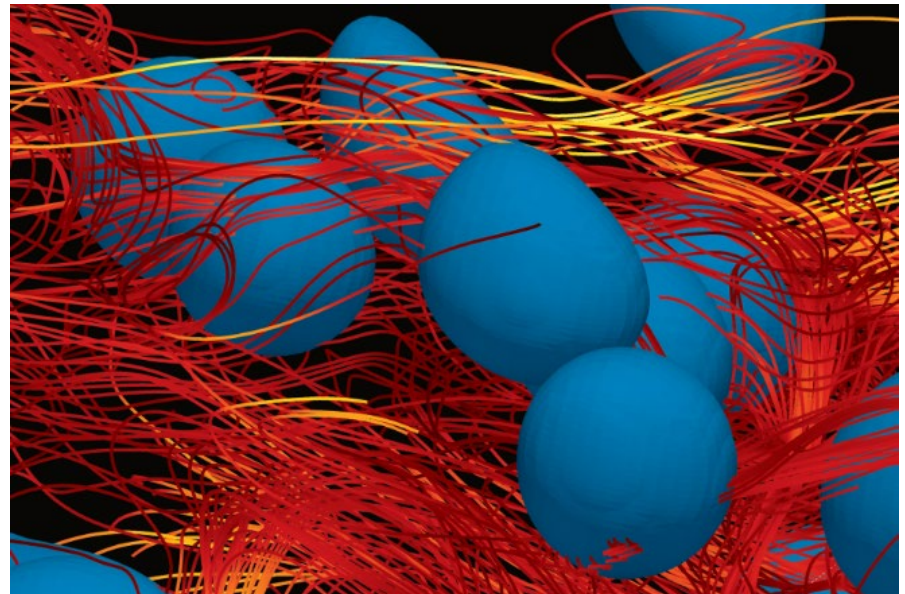
## Other Key Areas at TU Wien

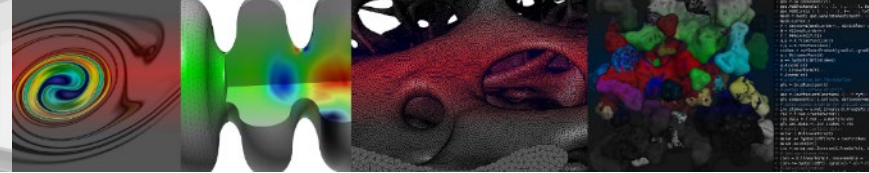
### Computational Fluid Dynamics & Acoustics

*... simulate fluid transport and acoustic phenomena*



Source: Soldati, TU Wien

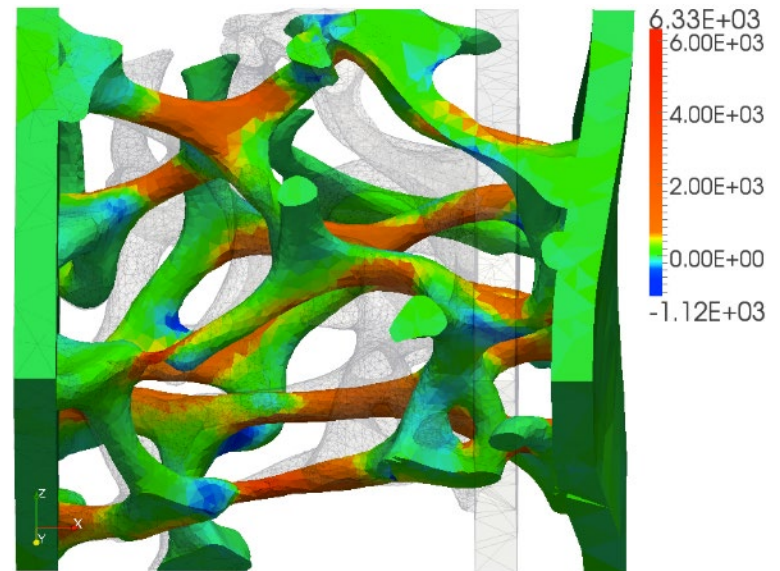
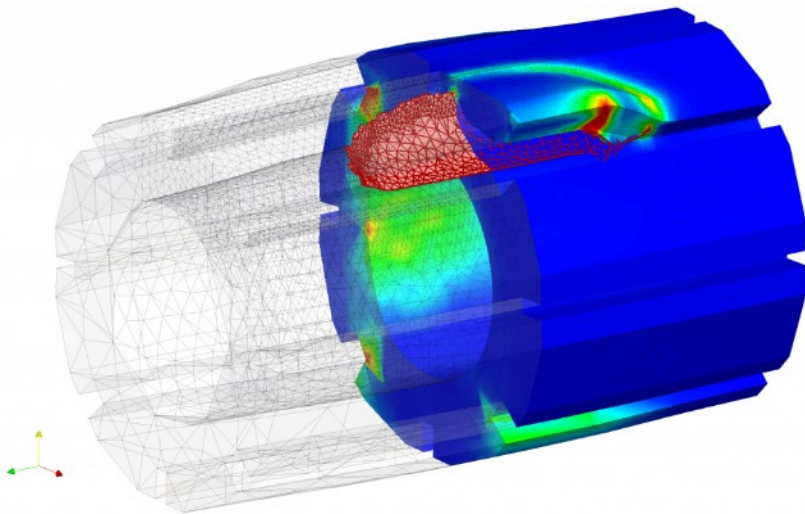




## Other Key Areas at TU Wien

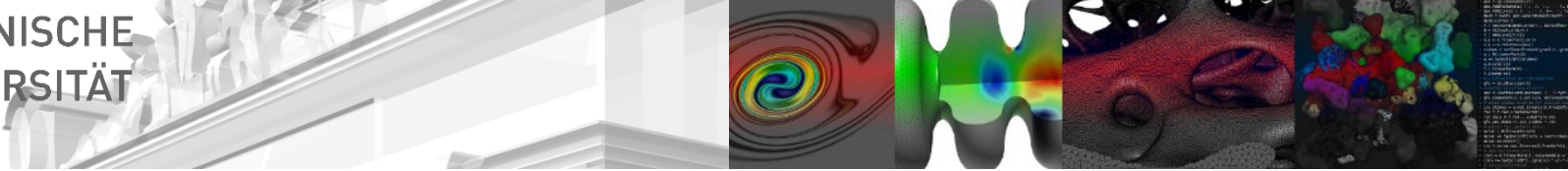
### Computational Solid Mechanics

*... simulate stresses and strains in solids*



Source: Pearce et al., Archie-West, University of Glasgow

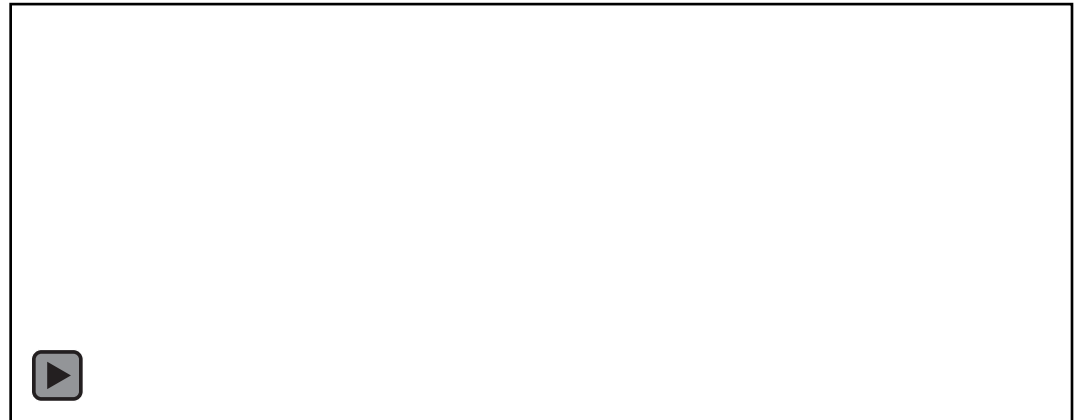
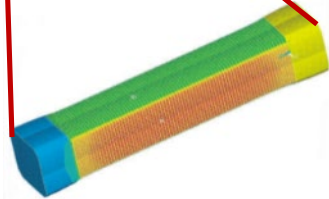
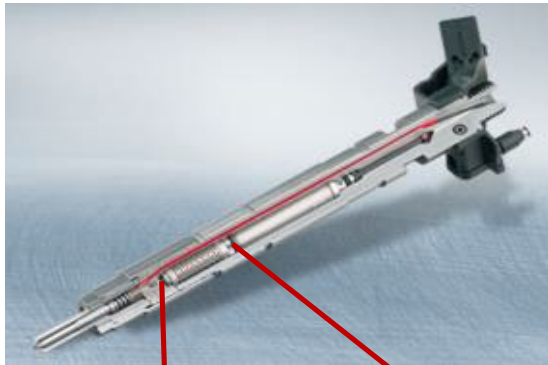




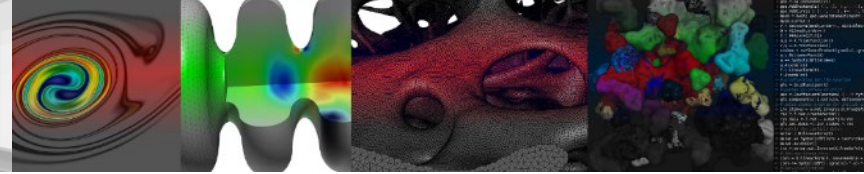
## Other Key Areas at TU Wien

### Computational Mechatronics

*... simulate electro-mechanical systems*



Source: Kaltenbacher, TU Wien



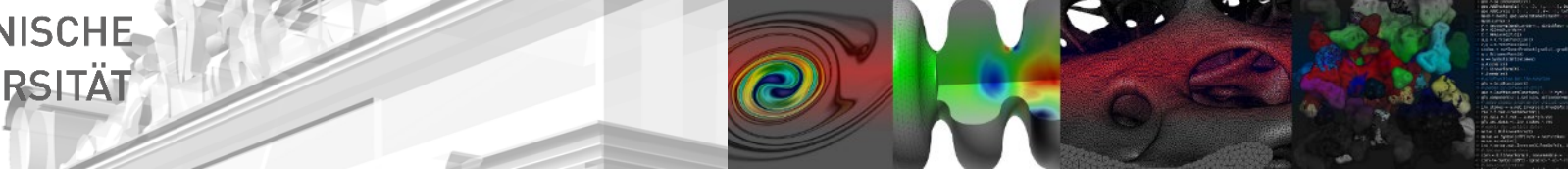
## Other Key Areas at TU Wien

### Computational Informatics

*... conduct data management and analysis and solve optimization problems*



Source: Tamir, Berkeley, School of Information



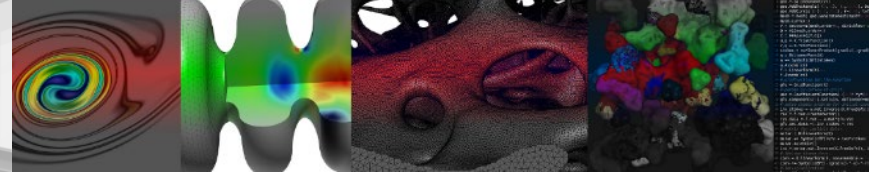
## CSE Master's Program Details

- Website (including extensive FAQs, German & English): [www.tuwien.at/cse](http://www.tuwien.at/cse)
- Email (central point of contact): [cse-master@tuwien.ac.at](mailto:cse-master@tuwien.ac.at)
- Four terms, 120 ECTS
- Master of Science (MSc)
- Admission: Graduates of the **technical chemistry bachelor's program of the TU Wien** are automatically eligible.

- **Interfaculty degree program**

Courses are held by experts from the following departments:  
(depending on the two key areas you select)

- Electrical Engineering and Information Technology
- Civil Engineering
- Informatics
- Mechanical and Industrial Engineering
- Mathematics and Geoinformation
- Physics
- Technical Chemistry



# CSE Master's Program Details

## Key Areas

2 × 15 ECTS

*Computational  
Building Science*

*Computational  
Chemistry and Materials Science*

*Computational  
Electronics*

*Computational  
Fluid Dynamics and Acoustics*

Select 2 out of 8

*Computational  
Informatics*

*Computational  
Mathematics*

*Computational  
Mechatronics*

*Computational  
Solid Mechanics*

each 15 ECTS

## Basic Modules

50 ECTS

**Computer Science**

17 ECTS

*Parallel Computing  
Programming*

**Scientific Computing**

15 ECTS

**Applied Mathematics**

18 ECTS

*Applied Mathematics Foundations  
Numerical Computation  
Numerical Partial Differential Equations*

## Electives & Thesis

40 ECTS

**Free Electives and  
Transferable Skills**

10 ECTS

**Master's Thesis and  
Defense**

30 ECTS

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