



Scientific-Software-Developer

APPLY NOW

Context

Our flagship product [GRACE](#) has been developed with and for our customers for over twenty years. From the early days up until today, we have been tightly connected to the experimental departments of large pharmaceutical companies, embracing their problems as ours.

We have pioneered and become the world-leader of [organic Crystal Structure Prediction](#). With our pharmaceutical industry customers and staff from all around the world, we are inventing the next generation of [software tools for in silico materials design](#).

We rapidly deploy new technology to leading pharmaceutical companies. We put the principles of sustainable development into practice and offer an industrial working environment with an academic touch.

Our offices are located in [Freiburg](#) (Merzhausen), Germany, on the border of the [Black Forest](#). The city has a rich student life with a variety of places to unwind after work. The residential areas offer [green](#), calm surroundings that are ideal for healthy lifestyles and families. Close to France and Switzerland, the Black Forest is one of Germany's most touristic regions known for the beauty of its lakes and landscapes. In the wintertime the region offers good opportunities for alpine and cross-country skiing.

Your responsibilities

You start in the next three months of the current year in a permanent position. You join a team of experienced Scientific Software developers and report to Dr. Marcus Neumann, the Science and IT Director and to Elsa Gheziel MA, the HR and Administration Director.

AMS' **GRACE** software is the most scientifically advanced software package for Crystal Structure Prediction (CSP). Depending on your interests and skills you will expand GRACE in various directions:

Computing Infrastructure

The cost of scientific computing matters to you. You would never compromise data security, but you know that there is a world of computing resources beyond your in-house LINUX cluster. By navigating through company networks and clouds to make calculations run on the most cost-effective hardware, you will push the limits of scientific computing.

Force Field Energy Calculations

You are a high-performance computing expert with experience in implementing force field technology for various hardware environments including GPUs. You will make our ab-initio grade force fields scale up to supercomputer size and perform close to the machine limit.

Machine Learning

You are a machine learning expert with a passion for atomistic modeling. Together with our domain experts you will introduce machine learning techniques in complex molecular modelling work flows to enable the next generation of industrial applications.

Crystallographic Computing

You admire the beauty of symmetry and group theory, but also appreciate the power of energy-aware crystallography. You will enhance modern crystal structure prediction by using information from crystallographic data bases and simulate experimental data from complex crystalline structure models.

Molecular Dynamics

You are a molecular dynamics expert and you have always wondered what your trade would be like with efficient ab-initio grade force fields. We have the force field. Go out and change the world of computational materials design by implementing high-value data flow processes and interfacing with third-party software.

Solubility Prediction

You have tried to predict the absolute solubility of pharmaceutical compounds by various means but never got close enough? We have a plan, you will contribute to making it work.

Crystal Nucleation and Morphology

You always thought that crystal structures deserve an interface? Our proven computational infrastructure and energy calculation methods will enable you to tackle the dynamic aspects of crystallization.

C++ Math Libraries

Linear algebra, derivatives, vectorization and optimization: you are willing to sacrifice neither performance nor the beauty of the library interface. Being an experienced C++ software developer knowing all the dusty corners of template libraries and inheritance, you will create the math libraries our scientific software depends on. You will also train new software developers on the C++ language.

Your profile

Soft skills: do you share our vision and values?

- You are committed to reduce the carbon footprint at work and care about Ethics in Business
- You are a team-player
- Can-do attitude
- You readily accept guidance by senior colleagues
- You are rigorous, precise and solution-oriented
- You can execute complex sub-projects independently
- You are pragmatic and willing to accept the constraints of a historically grown code
- You have a genuine interest in the development of efficient computer algorithms
- Intercultural awareness: our customers and teams come from all over the world. Thus, it is important to be able to adapt to different mentalities and cultural contexts

Hard skills: do you bring in...?

Both expert knowledge and hands-on experience in at least one of the domains mentioned in the “Your responsibilities” section.

- Object oriented and template programming in C++

- A strong molecular modelling background
- Fluent written and spoken scientific English

Education

Master in computer science, PhD in physics, chemistry, or a related field.

APPLY NOW

What we offer: a workplace to shape your future

We are a small family business with short communication paths. The impact of your work is immediately visible and directly supports other team members.

We aim to provide a professional environment in which people from all over the world at different stages of their lives can find the work-life balance that suits them.

Because we care about our employees, our customers' needs, scientific progress and the planet, working at AMS does have a meaning.

- Flexible work time management around core hours
- Free organic coffee & teas, fresh fruits
- Resilient, organic garden with a planter where employees can grow their own fruits and vegetables
- A quiet workplace with the quality of a living space (not open plan offices)
- Part-time work for some of the positions
- Job specific training
- Yearly: 28 days paid leave (full time based) + about 10 days public holidays
- Equal opportunity policy
- Help with settling in if you are located outside Germany

What about recruitment at Avant-garde Materials Simulation?

Avant-garde Materials Simulation Deutschland is an [equal opportunities](#) recruiter: your application is welcome regardless of your age, gender, ethnic origin, disabilities or

religion/beliefs.

What matters most to us, beyond your skills and experience, is your mindset. Tell us more about your philosophy at work and your soft skills in your application form under Your Motivation-s.

Step 1

Fill-in [Application Form](#), and you get notified in case of successful completion.

Step 2

Pre-screening of candidates by AMS Human Resources, and you get notified about early rejection, or Step 3.

Step 3

You are invited to take some hard and soft-skills tests, and you get notified about rejection, or Step 4.

Step 4

Remote interview, and you get notified about rejection, or Step 5.

Step 5

On-site day in Freiburg: series of hands-on tests and interviews with AMS Management and the concerned Department.

Step 6

Decision on job offer, you get notified within 2 weeks.

Curious?

Visit our website

Discover Avant-garde Materials Simulation Deutschland GmbH.
Sharing common values is the basis for a diverse and happy Team!



Our mindset

- We are addicted to innovation
- Our software is used by many large pharmaceutical companies
- Our customer's problems are our problems
- We are a family business
- We do business to invest in science, not the other way around

Our Business Ethics

- Sustainable development
- Renewable energies
- Soft mobility and CO2 offset for travels
- Low energy consumption
- A culture of respect and openness towards colleagues and partners