



PDC Application Experts

Code Optimization

Tor Kjellsson Lindblom
Theoretical & Computational Physics
(Ph.D., Stockholm University)



Previous research and work

- development of computational code to solve the time dependent Dirac (and Schrödinger) equation for atomic systems interacting with ultrastrong laser pulses, specifically treating effects beyond the electric dipole interaction
- implementation of analytical methods for light-matter interaction based on asymptotic behaviour of wavefunctions

Current work

- support and training for PDC users
- postdoctoral researcher at Oslo Metropolitan University: conducting research on relativistic light-matter interactions, including effects beyond the so-called electric dipole approximation, between ultrastrong near-infrared laser pulses and atomic systems

Can help PDC users with

- general debugging and code optimization, especially in FORTRAN but also Python and C++
- parallelization with OpenMP, MPI and hybridization strategies

Bioinformatics & Molecular Biology

Previous research and work

- bioinformatics research at AstraZeneca
- sequencing within the human genome project
- proteomics tool for data extraction/integration (github.com/percolator/pout2mzid)

Current work

- head of PDC HPC Support/Application Experts
- developing a gene-environment interaction analysis tool (bitbucket.org/menzzana/geipac)
- scientific manager for Tryggve, NeIC (neic.no/tryggve2)
- member of the SNAC working group

Can help PDC users with

- genetics, molecular biology, bioinformatics
- development for biological analysis tools

Henric Zazzi
Molecular Biology
(Ph.D., Karolinska Institute)



Molecular Dynamics

Thor Wikfeldt
Computational Chemistry & Chemical Physics
(Ph.D., Stockholm University)



Previous research and work

- molecular-level simulations of liquid, solid and surface systems using electronic structure, molecular dynamics, Monte Carlo, enhanced sampling and path-integral methods
- ab initio calculations of x-ray and neutron scattering spectra
- development of a hybrid force field based on polarisable electrostatics & many-body machine learning potentials

Current work

- instructor at CodeRefinery (coderefinery.org)
- PDC/SNIC training coordinator
- development of HPC training material
- application support for molecular dynamics and electronic structure software packages
- technical infrastructure at PDC

Can help PDC users with

- molecular dynamics and electronic structure codes
- modern HPC usage patterns (Jupyter Notebooks, HPC workflow management tools)

Our Application Experts at PDC (and those at other SNIC computing centres in Sweden) can assist you with research using high performance computing (HPC). These experts each have a research background in a particular scientific area, along with extensive experience using HPC applications in that area. If you would like assistance to use HPC in your research, please contact our experts: support@pdc.kth.se.

Multiscale Modelling

Previous research and work

- multiscale modelling of optoelectronic and magnetic properties of organic functional materials
- optimization of force field parameters for organic molecules and metal nanoparticles
- ab initio exciton model for efficient and scalable simulations of multichromophoric systems

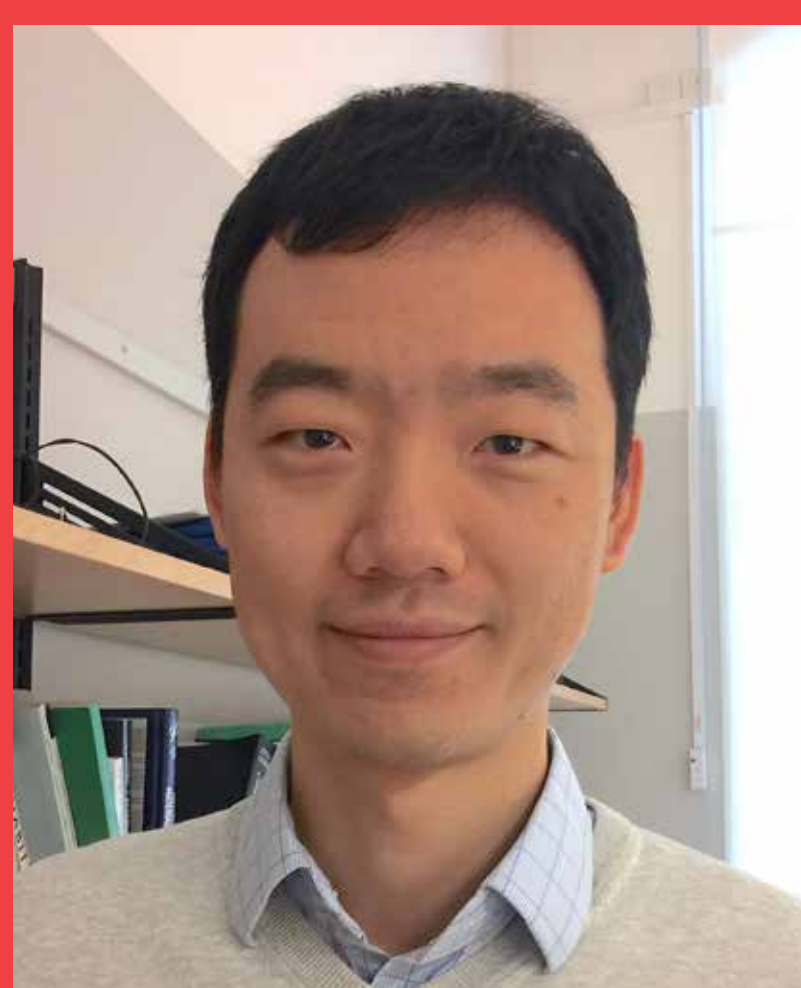
Current work

- hybrid simulation approaches for optoelectronic responses of biomolecules
- large-scale parallelization of quantum chemistry calculations
- benchmark & optimization of scientific computing codes
- support and training for PDC users

Can help PDC users with

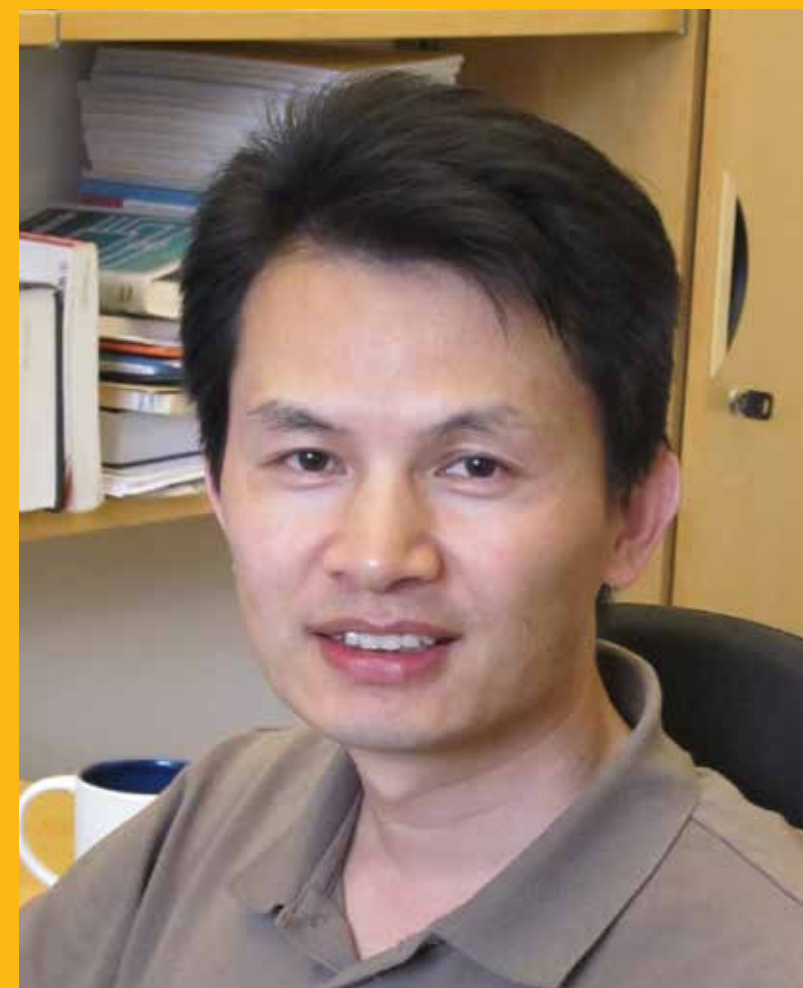
- general scientific computing problems
- troubleshooting scientific software
- parallelization of scientific computing codes

Xin Li
Theoretical Chemistry and Biology
(Ph.D., KTH Royal Institute of Technology)



Computational Fluid Dynamics

Jing Gong
Scientific Computing
(Ph.D., Uppsala University)



Previous research and work

- industrial FEM code development
- computational fluid dynamics in conjunction with the Department of Mechanics, Scania, and the Department of Aeronautical and Vehicle Engineering, KTH
- various EU research projects (such as ExaFLOW)

Current work

- computational fluid dynamics
- PRACE project
- Scania research collaboration project

Can help PDC users with

- computational fluid dynamics
- general scientific computing problems
- parallelization and optimization of code development

Machine Learning & Performance Analysis

Previous research and work

- design and implementation of scalable methods for performance monitoring and analysis
- development of parallel runtime systems
- analysis and optimization of parallel code

Current work

- support for PDC users
- performance analysis and benchmarking of parallel codes and infrastructures
- machine learning methods applied to performance data

Can help PDC users with

- deep learning/machine learning
- performance analysis of parallel code
- code parallelization and optimization

Xavier Aguilar
Computer Science
(Ph.D. candidate 2019, KTH Royal Institute of Technology)

