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Series Editor:
Felix Breitenecker (ARGESIM / ASIM)
Div. Mathematical Modelling and Simulation,
Vienna University of Technology
Wiedner Hauptstrasse 8 - 10, 1040 Vienna, Austria
Tel: +43-1-58801-10115, Fax: +43-1-58801-10199
Email: Felix.Breitenecker@tuwien.ac.at

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Editors: Inge Troch, Felix Breitenecker
Div. Mathematical Modelling and Simulation,
Vienna University of Technology
Wiedner Hauptstrasse 8 - 10, 1040 Vienna, Austria
Email: Inge.Troch@tuwien.ac.at

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ARGE Simulation News (ARGESIM)
c/o F. Breitenecker, Div. Mathematical Modelling and Simulation, Vienna Univ. of Technology
Wiedner Hauptstrasse 8-10, A-1040 Vienna, Austria
Tel.: +43-1-58801-10115, Fax: +43-1-58801-10199
Email: info@argesim.org; WWW: http://www.argesim.org

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HOW MATHEMATICS CAN SPEED UP QUANTUM MECHANICAL CALCULATIONS OF SOLIDS

K. Schwarz
Vienna University of Technology, Vienna, Austria

Corresponding Author: K. Schwarz, Vienna University of Technology, Inst. f. Materials Chemistry
Getreidemarkt 9/165-TC, 1060 Vienna, Austria; kschwarz@theochem.tuwien.ac.at

Introduction. Today rather complex materials can be simulated applying different methods according to the corresponding length scale. At the atomic scale, where the electronic structure plays the dominant role, calculations are mostly done with density functional theory (DFT) and often with the WIEN2k program package (see www.wien2k.at) that has been developed during the last 28 years and is used worldwide by more than 1400 users in academia and industry [1]. Mathematics can contribute a lot to achieve high efficiency; some important aspects are:

Material sciences. A solid (or surface) is represented by a unit cell and periodic boundary conditions. The cell is defined by its shape and the atoms it contains, which may be 1 or over 1000, where each atom is specified by its atomic number and the position in the cell. The properties vary from insulators, metals to magnets.

Electronic structure requires quantum mechanics, e.g. DFT leading to one-electron Schrödinger-type Kohn-Sham equations, which need to be solved iteratively within self-consistent field (SCF) cycles. From an input density one generates a potential leading to wave functions which define an output density. A clever mixing between input and output density (using a better than Broyden's mixing) can reduce the number of cycles. The wave functions are expanded in basis functions, which - in our case - are given in linearized augmented plane waves (LAPW). In order to find the expansion coefficients (according to the variational scheme) a general eigenvalue problem must be solved that is rather computing intensive (scales with n^3). The matrix size can be above n=50000. For the SCF cycles only the occupied states are needed and thus one can use a subspace and a modified Davidson solver using information from the previous cycles to find the necessary eigenstates.

Structure optimization. The atoms can move to their equilibrium positions till the forces acting on them vanish. A rough estimate of the Hessian (using results from previous steps) can reduce the number of steps towards the equilibrium geometry of the system.

Mathematics can provide efficient algorithms for the various tasks as indicated above. The mathematician must consider the specific needs of materials sciences but also the available computer architecture. In addition the numerical precision must often be very high, since the quantity of interest (e.g. the total energy) may vary in the eleventh decimal place.

Hardware and software. The rapid improvements in terms of in memory, communication, libraries, parallelization, etc need to be optimally utilized.

Summary. A high efficiency can only be gained by combining the expertise in all these fields. Optimization must consider which parts of matrices are dominant, how previous information can be reused but also numerical precision, convergence, data locality, band width, parallelization etc. These issues need to be addressed with proper algorithms, which recently were found to be very successful.

[1] Schwarz K and Blaha P.: *Solid state calculations using WIEN2k.* Computational Material Sciences 28, 2003, 259-273.