

# Quantum Wise

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## *ATK and VNL 2008.10*

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This release of Atomistix ToolKit and Virtual NanoLab not only provides a significant improvement in performance, but also marks the birth of a new company – QuantumWise A/S. As separately announced, QuantumWise has acquired all rights to develop and distribute these products from Atomistix A/S, which has ceased to exist. QuantumWise will also provide continued technical support for the software.

### *Highlights of this release*

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- Drastic performance improvement of 2–5 times
- Memory reduction of up to 50%
- Calculate 1,000 atoms on a laptop!
- ATK now threads/parallelizes on multi-core CPUs
- A new instrument in VNL: Bulk Builder

For more information, please see below.

### *Download it today!*

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To download the release packages, please visit <http://www.quantumwise.com/products/download>, where you will find more detailed information.

This release requires version **2008.10** (or later) of the **FLEXIm license features**. Users who have an active maintenance contract with Atomistix are entitled to a free license upgrade. Just contact [sales@quantumwise.com](mailto:sales@quantumwise.com) and we'll help you out!

QuantumWise is sincerely dedicated to further development and improvements of ATK and VNL, and hope that all existing – and new customers – will enjoy this and future releases. We truly believe ATK is the best code on the market for DFT calculations of large systems – and of course for transport studies!

*Copenhagen, December 2008  
The QuantumWise Team*

## New in Atomistix ToolKit 2008.10

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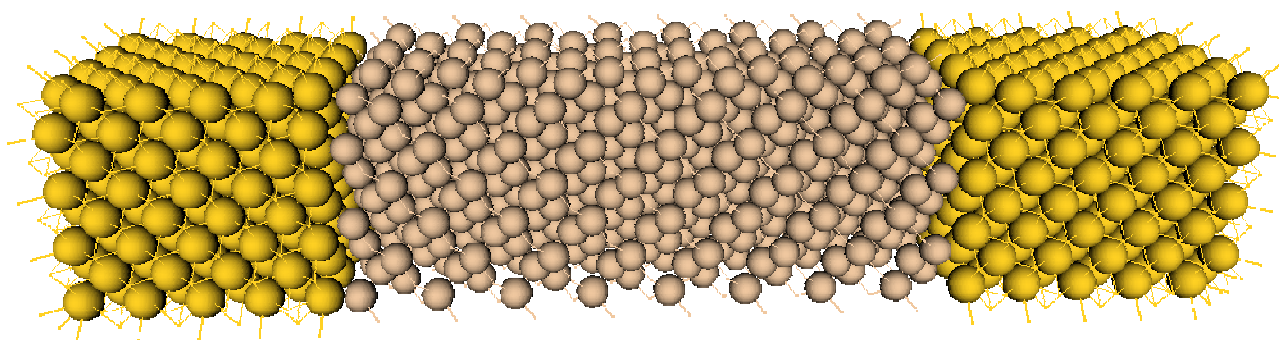
Many situations in life force you to choose between incompatible desires. If you want a fast and powerful car, you cannot really find one which also consumes very little fuel. With the latest edition of Atomistix ToolKit (ATK), version 2008.10, you can however have both!

With this release, the raw speed of the software has been improved by as much as 5 times compared to the previous version. At the same time, the memory consumption has been reduced to a level such that systems for which first-principles studies previously were only tractable on supercomputers with hundreds of nodes, are now possible to calculate on moderate sized clusters or even single multi-core workstations.

This pushes the limit of how realistic systems that can be treated, something which is not least crucially important when it comes to the influence of defects or impurities, in the quest for both novel electronic devices and catalytic processes, for example.

As an example of the extraordinary combination of performance and memory, a bulk MgO supercell with 1,024 atoms, converges in 16 hours on a single node, using just above 3 Gb of memory for a high-quality basis set (double-zeta polarized).

Or, if we focus on the unique capability of ATK to calculate transport properties such a current-voltage characteristics of nanoscale systems, a densely packed transport system with 1,166 atoms (Si and Au, see figure below) can be computed in less than 24 hours on 10 parallel nodes. The computation uses less than 2 Gb of memory per node with a single-zeta basis set, which means it could in principle be run on a laptop!

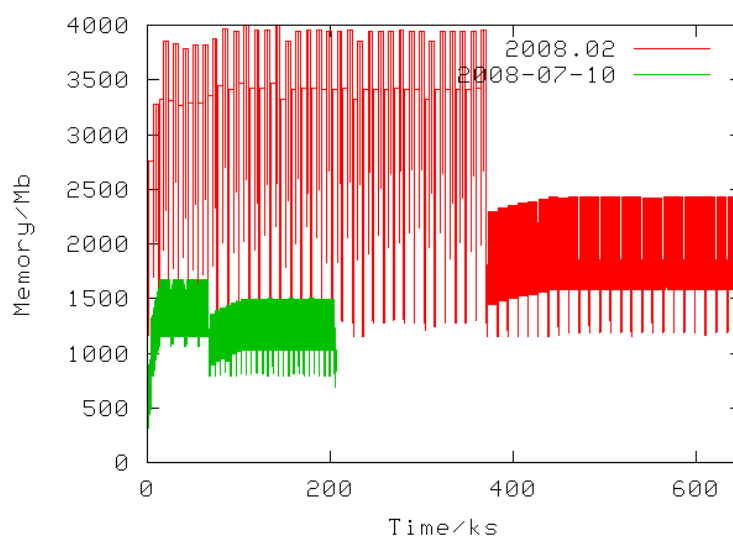


The memory and speed improvements are clearly demonstrated in the table below!

System	Speed-up	Memory reduction
Azafulleroid (molecule, 97 atoms)	1.1	15%
6x6x6 MgO (bulk, 432 atoms, Gamma point)	3.5	38%
6x6x6 MgO (k-point sampling (2,1,1))	2.3	32%
8x8x8 MgO (bulk, 1,024 atoms, Gamma point)	5.4	63%
AuSiAu (two-probe, 1,166 atoms*)	3.2	50%

\* 782 atoms in scattering region, 1,166 in equivalent bulk

In this table, the speed-up measures how many times faster the new version is compared to 2008.02 (a factor 2 means twice faster), while the memory reduction is given in percent (50% means half the memory).



*The improvements in memory usage and performance in ATK 2008.10 compared to 2008.02 are quite vividly demonstrated by this graph. This is a two-probe calculation for the system with 1166 Si and Au atoms illustrated above. The two distinguishable regimes (breakpoint at 350 ks for the red curve) are the equivalent bulk run and the two-probe calculation, respectively.*

To be specific, the performance upgrade is primarily due to three factors:

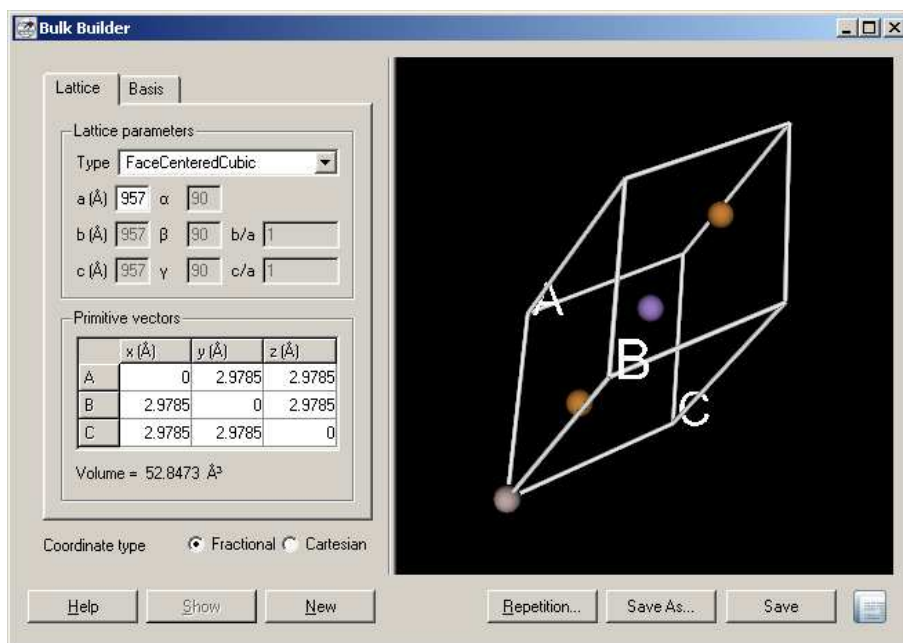
- The use of real matrices for Gamma-point sampling gives a very large performance boost for bulk systems and the equivalent bulk run of a two-probe system. Obviously, this does not affect systems with more than one k-point, but for very large systems a single k-point tends to be sufficient in many cases.
- The use of optimized libraries (specifically, Intel MKL), improves performance for all matrix operations, which not least is important for two-probe systems and large systems in general. These operations also parallelize on multi-cores.
- Tuned code. We have been over every single performance-critical part of the code and optimized them as best as possible, both for memory and speed, including compiler settings for each specific platform.

The introduction of Intel MKL also means that ATK now parallelizes over cores (threading) to take maximal advantage of e.g. dual-core architecture. For more information about this, please see the manual.

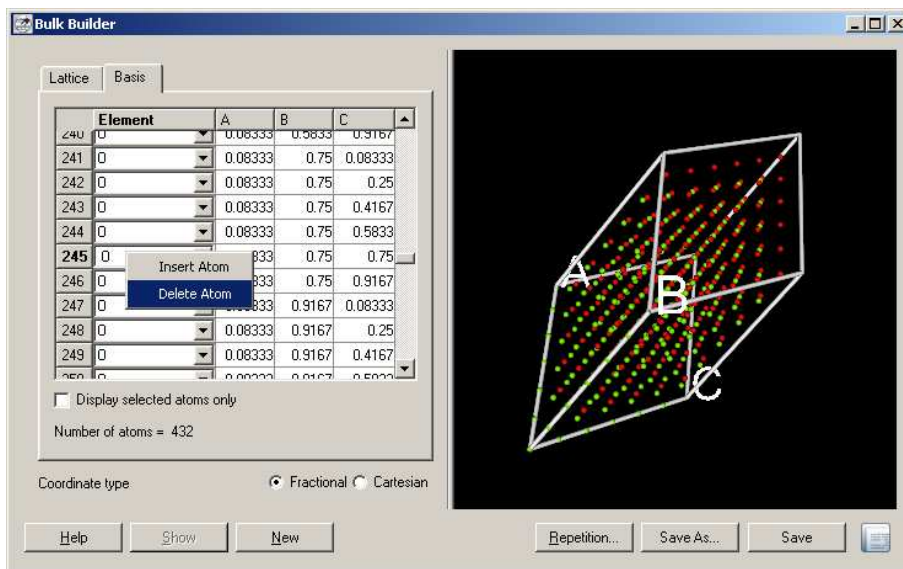
A few bug fixes are also introduced, although none are of major magnitude except one relating to calculation of the effective potential and electron density from a restored checkpoint files, which sometimes did not produce identical results compared to if you performed the calculation in the same script as the self-consistent loop.

## New in Virtual NanoLab 2008.10

In addition to this, we are also happy to announce a new instrument in Virtual NanoLab 2008.10: a **Bulk Builder**. It can be used to build bulk crystals or periodic atom configurations from scratch, or you can manipulate existing ones, including those found in the Crystal Cupboard. It is also possible to make supercells by repetition of the unit cell.



The Heusler structure AlMnCu, extracted from the Crystal Cupboard, open for editing in the new Bulk Builder instrument.



A 6x6 supercell of MgO (432 atoms) with a single defect (and oxygen vacancy) can very easily be built in the Bulk Builder by using the "Repetition" tool, and after that simply removing a single oxygen atom.