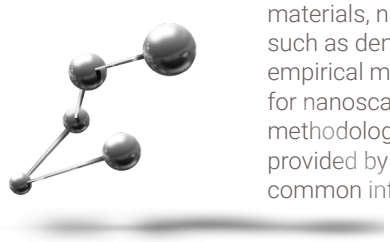
SYNOPSYS®

ATK-VNL Release Features
Version 2014

Last amended: June 2014



ATK-VNL 2014

ATK-VNL is a leading industry-proven platform for atomic-scale modeling of materials, nanostructures, and nanoelectronic devices. It includes quantum mechanical methods such as density functional theory (DFT) with either LCAO or plane-wave basis sets and semi-empirical models, simulation engine for atomic-scale simulations using classical potentials, module for nanoscale device and transport simulations using non-equilibrium Green's function (NEGF) methodology. ATK-VNL combines the power of a Python scripting engine with the ease-of-use provided by an intuitive graphical user interface, Virtual NanoLab. All simulation engines share a common infrastructure for analysis, ion dynamics and parallel performance techniques.

ATK-Classical

A New Module for Empirical Potentials and Molecular Dynamics (MD) Support

- **Over 160 bond-order potentials included, of many different types, allowing for advanced simulations of a wide variety of materials, including metal and semiconductor alloys, glass structures, and organic materials!**
  - Two/three-body potenitals: Lennard-Jones (various versions), Sutton-Chen, Stillinger-Weber
  - Tersoff (many versions)
  - Tapered potentials: Morse, Buckingham, Vessal, Tosifumi, damped dispersion
  - ReaxFF
  - EAM (fs+alloy)
- **Coulomb solvers: Ewald (smooth particle mesh), DSF, Debye, simple pairwise easy to add your own or other literature potential (of any of the above types) via a few lines of Python code.**
  - Support for custom combinations of potentials, like using a Stillinger-Weber potential with a Lennard-Jones term to account for van der Waals interaction.
  - This also makes support for literature potentials easy, like Pedone, Guillot-Sator, Marian-Gastreich, Feuston-Garofalini, Matsui, Leinenweber, ... (See the reference manual for details on each potential type)
- **Parallelized via OpenMP threading (also for ReaxFF)**
  - Up to 10x speedup on 16 cores
  - MPI parallelization with spatial decomposition scheduled for 2015
- **Advanced geometry builders**
  - Polycrystalline builder, using Voronoi tesselations
  - AFM tip builder
- **Property analysis and plotting (these are all available for DFT and DFTB as well)**
  - Local structure analysis (Voronoi type, centrosymmetry, partial charges)
  - Local stress
  - Elastic constants
  - Radial distribution function, velocity/kinetic energy distribution
  - Compute and visualize phonon vibration modes
  - Make movies (also for NEB paths)
- **MD methods**
  - ReaxFF
- **Set zero center-of-mass velocity explicitly**
- **Advanced monitor "hook" functions which make it possible to run e.g. stress/strain simulations**

So, you can think of this as very similar to LAMMPS… but a bit more:

- **Easy interface to define own potentials and combine potentials**
- **Device geometries - run NEGF thermal transport calculations**
- **GUI for building, setting up, and analyzing the results**

And as if that was not enough - there is now LAMMPS support in VNL! Import LAMMPS trajectories to make movies, calculate local structure, RDF, etc. Check the VNL for LAMMPS tutorials page!

Note 1: In order to run calculations using ATK-Classical and to use the Builder modules, you must have an ATK-Classical feature in your license file. This license is provided free of charge, upon request, for academic customers, and can be purchased as part of a commercial license.

Note 2: ATK-Classical is developed in collaboration with Fraunhofer SCAI under the Eurostars project ATOMMODEL.

Noncollinear Spin and Spin-Orbit Interaction

Originally introduced in ATK 13.8, the noncollinear features have been improved substantially, not least to achieve better convergence and accuracy. With the addition of spin-orbit interaction, you can now compute properties of e.g. topological insulators and - in combination with MGGA - get a good valence band structure of semiconductors.

- **Full noncollinear support for all DFT exchange models in ATK (LDA, GGA, MGGA)**
- **Also availble for Slater-Koster tight-binding calculations**
- **Support for bulk (and confined) periodic structures, as well as transport/device geometries**
- **Convergence trick: start from collinear converged result, by rotating density matrix in spin space**
- **Compute**
  - Magnetic anisotropy
  - Electron transport in magnetic tunnel junctions
  - Spin torque transfer (STT)
- **Spin-orbit coupling added for bulk (and confined) periodic structures, as well as transport/device geometries**
  - DFT: support added via OMX pseudopotentials
  - Semi-empirical tight-binding models: spin-orbit split parameters added for all built-in models
  - Spin-orbit split can also be set for DFTB models

New Features for Semiconductor Problems

- **New MGGA library and implementation - now also with TPSS functional**
- **New tutorial for details on how to calculate the band structure of InAs with a band gap and effective mass that matches experiments! The tutorial also presents two other new features:**
  - New tool for passivating dangling bonds on semiconductor surfaces, with detailed control of hybridization and bond lengths.
  - Fractional hydrogen atoms for passivating polar surfaces, like III-V nanowires and slabs
- **Effective mass tensor analysis - compute the band curvature at arbitrary k-points (not just extrema) and project along various directions for accurate values of the effective mass**
- **Doping is very important to study realistic semiconductor devices. However, if you attempt to use explicit dopants (which of course always is possible), the resulting doping concentration will be very high, or you need very large supercells. In ATK you can now introduce an additional ion charge of a region of atoms to simulate doping of that region.**
- **New in 2014, compared to 13.8 (and some preview versions of 2014):**
  - "charge" is now net charge (thus, normally just keep it zero)
  - Doping via atom indices no longer works – use tags!

Computational Performance Improvements

- **New MKL/compiler gives 35-40% general speed-up**
- **Improved speed of multigrid method**
- **Sparse storage of self-energies**
  - Optional reduction of memory overhead by storage of selfenergy by truncating small numbers
  - High gain for systems with band gaps in the electrodes. Little gain for metals.
- **Sparse recursion self-energy calculator**
  - Very large memory gain for short range basis sets (like Slater-Koster tight-binding), little or no gain for long-rang basis sets
- **Parallel Poisson solver ("direct solver")**
  - Constant time solving of the Poisson equation - significant
- **Sparse eigenvalue solver for diagonalization (FEAST)**
  - High gain for large basis sets, no gain for small basis sets
- **Optimized blocking and orbital sorting**
- **Tetrahedron method made faster for DOS**
- **A reminder for all users: set OMP_NUM_THREADS=1 if you place several MPI processes on the same node, else parallel performance degrades substantially.**

Graphical Performance Improvements

By rewriting our graphics engine to use advanced techniques otherwise employed in 3D games, like OpenGL shaders, the graphical performance of VNL has been improved to provide state-of-the-art rendering capabilities.

- **The Viewer and Movie Tool can now render millions of atoms fluently (without bonds). The Builder will be upgraded in 2015 to same capacity, for now it handles 10,000 atoms easily**
- **This technology requires modest hardware – OpenGL with shader support is available even on common onboard cards like Intel HD 2000 and is supported in both Windows and Linux**

New VASP Features

VNL is not only a GUI for ATK. In principle, users can write plugins to support any other atomic-scale modeling code, and to demonstrate this we have added an extensive suite of filters which turn VNL into a GUI for VASP.

Already in VNL 13.8 it was possible to create input files for a VASP calculation, using the VASP Scripter. This has been extended with support for band structure calculations, plus a few other updates. The tool gives a graphical interface to almost all common VASP settings, and produces ready-to-run input files, incl. POSCAR, POTCAR, KPOINTS, and INCAR.

New in 2014 is the possibility to also analyze VASP output files. With a simple click on EIGENVALS you can plot a band structure, project the density of states from DOSCAR on different angular momenta, visualize a 3D grid like the electron density (CHGCAR or PARCHG) or effective potential (LOCPOT), and even make movies from relaxation trajectories (CONTCAR), NEB or MD trajectories (XDATCAR). You can also benefit from the general tools in VNL to e.g. subtract two densities from each other or project a 3D grid onto a line through the cell, for instance to show the potential as function of Z, averaged over the XY plane, for a slab calculation.

Other Codes

Similar features are also added for other codes:

- **QuantumEspresso: configurations, energies, stresses, forces, charge densities**
- **GPAW: configurations, trajectories**
- **Materials Studio: XTD files**
- **LAMMPS: trajectories**

More will follow in future releases, and we encourage our users to suggest codes or data sets that should be supported!

New General Features

- **Export animated GIFs from movies**
- **Generate auto-rotated movies**
- **LDOS for semi-empirical models**
- **Many new basis sets from OpenMX + FHI, with support for DFT spinorbit**
- **Repetitions in Viewer (atoms and bonds)**
- **New or updated plugins (LabFloor)**
  - Cube file export, also for complex grids and with configuation included
  - GridOperations – subtract and add grids easily
  - Electrode validator
  - I-V curve shows show spin up/down currents

- **Spatial regions handling in Builder improved**
  - Specify regions in fractional coordinates
  - Translate regions
  - Keyboard shortcut to hide/show (R)
- **Plugin enhancements (Builder)**
  - Niggli tool for reducing crystal cells to basic form
  - Translate, rotate, mirror for NEB
  - Device from bulk improved
  - “Repeat” retains crystal symmetry (when possible)
  - Copy lattice parameters easily
  - Extract an image from a NEB configuation
- **General LabFloor**
  - File handling performance and stability improvements
  - Quickly unselect all files
- **Preferences dialog**
- **API updates**
  - Toolbar plugins in Viewer
  - read_state=False – just read metadata, not entire data, also for analysis quantities
- **Added menus for common keyboard shortcuts and basic operations in Builder/Viewer**

Updated Editor

- **Search/replace**
- **Code completion and highlight**
- **Syntax popup help**

Low-Level Entities

It is now possible to directly access a lot of “internal” low-level ATK quantities in Python:

- **Hamiltonian and overlap matrices**
- **Density Matrix**
- **Self energies**
- **Retarded Green’s function + left/right Green’s function**
- **Dynamical matrix and overlap**
- **Phonon self energies**
- **Phonon retarded Green’s function and left/right phonon Green’s function**

With these you can implement a lot of cool stuff yourself - some examples like 4-terminal transport and AC conductance are given in a tutorial!

Native Mac OS X Version

ATK and VNL now run natively on Mac! (OS X 10.8 or higher is required).

Other Improvements and Additions

- Limited memory Broyden–Fletcher–Goldfarb–Shannon (LBFGS) is new default optimizer
- Grimme DFT-D2 reimplemented in C++ (Python was too slow for large systems)
- Reduced package size by 30-40% by only shipping one Python library
- Packages added: SciPy, Scalapack, Blacs
- Fundamental constants in ATK updated to CODATA 2010
- Added lastImage() method to optimization trajectories too
- Export band structure includes actual k values for data points
- OpenSSL support (e.g. to connect to https databases)
- Improved error messages for license problems

Bugfix Update VNL-ATK 2014.0

No serious bugs in the calculation engine are known from previous version of ATK (going back to ATK 12.8). The following are however real issues that were fixed:

- Corrected stress projection – could cause optimizations to converge very slowly or to wrong cells
- Setting the number of Fermi function poles did not have any effect (note that this is an important convergence parameter/trick!)
- Reading and writing large structures (20,000 atoms and more) to/from NC files was very slow (this also made VNL slow when transferring such structures between Builder, Scripter, Viewer, etc)
- Viewer
  - Corrected unit for grids
  - Isosurfaces now showing correct min/max
  - I-V curve, negative bias going in the correct direction now
  - Horizontal axis of phonon DOS was eV, should be meV
- Sort coordinates fixed for large systems (also influenced device from bulk!)
- Conflict with IPython fixed
- Better support for setuptools in ATKPython
- Other smaller bugs, mostly cosmetic
- VASP PDOS would not display correctly
- POSCAR/POTCAR export was not in sync, resulting in incorrect structures
- Effective mass widget, conversion between fractional and Cartesian directions was wrong
- Cylindrical spatial regions did not always render correctly on Windows
- Move tool did not work on some non-NVIDIA graphics drivers
- Added support for shader graphics on Intel HD 4000 graphics cards
- libGLU, proper pre-loading
- Conflict with existing Qt libaries on some Linux distributions fixed
- Some scripts and NC files in the Example project did not work properly
- Axis labels in 1D Projector corrected
- Literature references for ATK-Classical corrected
- Fixed graphics problems on Fedora 15 (32-bit)
- Better reporting of OMX basis sets in the General Info plugin
- Builder view not always updated correctly when switching projects
- FHI-AIMS is not available on 32-bit platforms, and now there is a proper error message about that
- nlprint problems for some objects (like DOS) when using spin-orbit or noncollinear spin fixed

Outstanding Bugs and Known Issues

At the moment we are not aware of any bugs in ATK/VNL that would influence the results or significantly disrupt the operation of the software. We are working on improving the graphical performance of VNL for large-scale systems (100,000+ atoms) and the new prototypes we have are already 2x faster in computation time for some parts, and also scale much better in parallel, so stay tuned for another great version to be released in 2015! We are also investigating the following points:

- **VNL fails to start unless the "bin" directory is in your path - workaround: add the directory to your path, or change the "Start in" folder for the Desktop/Start menu shortcut to the "bin" folder (fixed in 2015)**
- **VNL can crash if you click the Builder icon while a large configuration is being loaded - temporary solution: don't.**
- **Problems with mixed-version nc files - take care not to "nlsave" into existing NC files of older versions. This is not really a bug, it's simply how it's designed, but it can cause some unexpected behavior.**
- **Ghost atoms are rendered as usual atoms (but without bonds) in shader-based graphics, rather than wireframe as otherwise (fixed in 2015).**

Bugfix Update VNL-ATK 2014.2

The numbers in parenthesis are our internal issue tracking numbers, listed here just for our own reference.

Serious Bugs

- **Calling evaluate() on TransmissionEigenvalues multiple times gave different results, because the underlying C++ object was corrupted by evaluate() itself - fixed (7950)**
- **Work-around for MKL bug in FFT2D with grids containing 2n grid points (7701)**
- **Long MD trajectories could not be viewed due to memory problems - fixed (7704)**
- **Phonon band structure were calculated wrong for structure with negative coordinates (7729)**

Bugs (Infrequent or Not Affecting Results, But Annoying When You Hit Them)

- **EffectiveMass Analyzer showed incorrect band index (7684)**
- **Specified doping (actually, atomic compensation charges) is now kept when increasing the size of the central region in a device (7479)**
- **Nanoribbons and nanotubes generated in the Builder are now BulkConfigurations (instead of special classes, which tripped up plugins and drop events) (8141)**
- **Abinit failed to run when the configuration contained too many atoms (7492)**
- **Selection in DOS visualizer with noncollinear and spin-orbit fixed (8178)**
- **Maximum number of eigenvalues for noncollinear/spin-orbit in DensityOfStates+Bandstructure fixed. Caused problems using the bands_above_fermi_level argument (7477, 7943)**
- **Classical potential class EAM_HPd_2008 fixed - filename reference was wrong (8183)**
- **Fixed issue with nlprint for EffectiveMass for Cartesian directions (7675)**
- **ExpressionSelect (Builder) handles incorrect expressions better, instead of just selecting all atoms (7947)**
- **Modified the threshold for two-probe device checks - older version caused problems for very long devices due to rounding (7909). This issue may not be 100% fixed, but you have to use very long devices to see it.**
- **OpticalSpectrum no longer reports spin up and down separately for the dielectric constant (which makes no sense); notes added to the Reference Manual also (7969)**
- **Command line shortcut now makes certain to run the correct "atkpython", even if you have several versions installed (7677)**
- **The "c" parameter is now properly kept when dropping a Meta-GGA configuration on Scripter (7705)**
- **Symmetry labels now remain in the band structure plot when you set the axis limits using the Customize dialog (6899)**

Minor Bugs (Hardly Noticed or Very Infrequent)

- y axis label was wrong for ExchangeCorrelationPotential in Projector1D (7678)
- Builder did not respect “exclusive mode” any more, so you could “fall out” of the Move tool for instance (8004)
- Files added to project subdirectory were not properly selected and loaded (7914)
- Fix for filename in IVGenerator (7806)
- Fix for k-point symmetry errors in cases when ghost atoms and normal atoms of the same element have different basis sets (7948)
- Fix for Mac OS X MDI problems in the Viewer (7520)
- JobManager - disabled starting of queue, when something is already running (7702)
- Improved messages in the Electrode Validator (7683)
- Legend now updates automatically when changing curve labels in the 1D Projector (7493)
- Rare error in license system when the locale is not set correctly on Linux fixed (8008)
- Removed line/point pickers for log-scale axes (7714)
- Some inconsistencies in spin handling for spin-orbit fixed (7511)
- Some SelfEnergyCalculator flags were not saved/restored properly in the Script Generator (7913)
- Unsupported elements are now properly reported as such in the Script Generator (problem appeared for Gd for instance) (7960)
- When the last stash item was deleted, it remained in the 3D view (when using shaders) - fixed (2981)
- When you zoomed quite far into band structure plots, the plot points would disappear - fixed (7297)
- A spurious bond could remain when deleting an atom in the Builder in special cases (8192)
- OpenGL problem on (k)ubuntu 10.04 solved (7330)

Improvements

Not everything that doesn’t work as intended is a “bug” - sometimes we just don’t have time to implement everything at once

- Several updates to the VASP plugins, to support more cases found in DOSCAR and EIGENVAL files (e.g. Cartesian k-points, or various types of projections), and for MD Trajectories with NWRITE=2. (7718, 7733, 7791, 7669, 8206)
- Improvements to parsing QuantumEspresso files (7949, 7534)
- Enabling StillingerWeber_BN_2005 potential again (8183)
- Better handling of view settings when using “repeat” and “undo” in the Builder (7706)
- Added license config to installer (7998)
- Improved memory usage esitmate for noncollinear calculations (7934)
- Visualization of FHI-AIMS density of states objects enabled (7039)
- Better sorting of database search results (7464)
- Improved CIF parser, to import files with “:” in the HM symbol - also gives better error messages when it fails (8003)
- Memory usage widget fixed (appeared behind other windows, and on Mac OS could not even be moved in front of the New Calculator widget) (7465)
- Removed GUI code from the passivation code, so it can be used in a script (7588)

Outstanding Bugs and Known Issues

At the moment we are not aware of any bugs in ATK/VNL that would influence the results or significantly disrupt the operation of the software. We are still working on improving the graphical performance of VNL for large-scale systems (100,000+ atoms) and the new prototypes we have are already 2x faster in computation time for some parts, and also scale much better in parallel, so stay tuned for another great version to be released in 2015! We are however alerted of the following points (besides very exotic and minor stuff):

- **VNL can crash if you click the Builder icon while a large configuration is being loaded - workaround: don't**
- **Problems with mixed-version nc files - take care not to "nlsave" into existing NC files of older versions**
- **Ghost atoms are rendered as usual atoms (but without bonds) in shader-based graphics, rather than wireframe as otherwise - fixed for 2015**
- **The font color is set to the background color in interactive mode sometimes on Windows 8. No workaround available for now.**

Also, we had intended to make VNL 2014.2 start up properly on Windows without the need to have the "bin" directory in the PATH (or set as "Start in" folder for the Desktop shortcut) but that didn't work. So, you still need to either have it in your PATH or modify the Start in folder. The installer actually adds it to the PATH automatically, but in case someone else installed VNL on your machine, you may need to add it manually.

Bugfix Update VNL-ATK 2014.3

- **Spin-orbit, spin-polarized and non-collinear models corrected and improved**
  - Updated how all 3D grid objects are handled w.r.t. spin for consistency and correctness. For instance, you no longer specify the spin parameter when you compute the grid, only when you query it (via the evaluate method).
  - Spin-orbit model for selfconsistent semi-empirical Slater-Koster and Huckel corrected
  - Correctly handle the imaginary UPUP/DOWNDOWN part in sparse Fourier transforms (8975)
  - Spin-polarized electron density for the extended Huckel model corrected (10104)
  - Fixed non-collinear dense transmission coefficient (now L->R) (9318)
- **Fix for DeviceDensityOfStates with spin-orbit (9027)**
- **BSSE and Grimme now work together**
- **Neumann boundary conditions for FFT2D**
  - Fixed for bulk configuration (9186)
  - Disable double Neumann in any direction (9231)
- **LocalStress, several bugs fixed**
- **nlsave/nlread MGGA-TB09 calculations now saves and restores the "c" parameter properly (9430)**
- **Effective mass now requires that you specifies a direction, i.e. we no longer compute the tensor and then project, since this doesn't work for degenerate bands**
  - Also corrected the fractional coordinate in the report
- **Improved error message for phonon calculations using semi-empirical models without a pair potential (9513)**
- **1D projector constant CPU usage fixed (9226)**
- **Restart polarized calculation from unpolarized initial state (9418)**
- **Fixes for bands_above_fermi_level in Bandstructure/DensityOfStates (8987)**
- **Make GridValues.evaluate/derivatives always return a PhysicalQuantity (10062)**
  - ATK-Classical/TremoloX
  - Bugfix for potentials with tags
  - Corrected a parameter in the Oligschleger_Se_1996 potential
  - Minor updates in the ATK-Classical plugins
  - Fixed small error in the reference manual for the Morse potential

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