Many application areas in nanotechnology are related to effects occurring at junctions, interfaces, and surfaces. It is critical to be able to accurately model such phenomena from quantum theory. QuantumWise offers unique software tools for these systems, centered around an open platform architecture.
QuantumWise offers a software platform for atomistic simulations of nanoscale systems

- **Atomistix ToolKit** (ATK)
  - State-of-the-art DFT engine for electronic structure and transport calculations

- **Virtual NanoLab** (VNL)
  - Modern GUI for setup and analysis

- **NanoLanguage**
  - Scripting language interface to ATK
  - Fully integrated in VNL
Examples of application areas (1/2)

- Current-voltage characteristics of molecular junctions and tunneling devices (rectification, NDR)
- Contact resistance and capacitance of metal-nanotube and nanotube-nanotube contacts; Schottky barrier
- Current-voltage characteristics of functionalized carbon nanotubes
- Graphene field-effect transistor
Examples of application areas (2/2)

Spin-dependent transport across crystalline magnetotunnel junctions

Leakage currents in MOS structures
High-k dielectrics, complex interfaces

Reaction paths on surfaces for catalysis

Defect states in semiconductors, nanowires, nanotubes
Selected publications 2008-2009 with ATK

**Graphene**
- OuYang et al., *Transport properties of T-shaped and crossed junctions based on graphene nanoribbons*, Nanotechnology 20, 055202 (2009)
- Lam et al., *An ab initio study on energy gap of bilayer graphene nanoribbons with armchair edges*, APL 92, 223106 (2008)
- Li et al., *Role of symmetry in the transport properties of graphene nanoribbons under bias*, PRL 100, 206802 (2008)
- Sevincli et al., *Superlattice structures of graphene-based armchair nanoribbons*, PRB 78, 245402 (2008)

**Nanotubes**

**Spintronics** (incl. graphene and nanotubes)
- Min et al., *CrAs(001)/AlAs(001) heterogeneous junction as a spin current diode predicted by first-principles calculations*, J. Mag & Mag Mat 321, 312 (2009)
- Sekiguchi et al., *Observation of a bias-dependent constrained magnetic wall in a Ni point contact*, PRB 78, 225518 (2008)
Selected publications 2008–2009 with ATK

**Molecular electronics**
- Fan et al., *Theoretical investigation of the negative differential resistance in squashed C_{60} molecular device*, APL 92, 263304 (2008)
- Zhao et al., *A possible anthracene-based optical molecular switch driven by a reversible photodimerization reaction*, APL 93, 013113 (2008)

**Nanowires**
- Ng et al., *Geometry dependent I-V characteristics of silicon nanowires*, Nano Letters 8, 3662 (2008)
- Yang et al., *Compositional ordering and quantum transport in Mo_{6}S_{9-x}I_{x} nanowires: Ab initio calculations*, PRB 77, 165426 (2008)
- Zhou et al., *First-principles study on the differences between the equilibrium conductance of carbon and silicon atomic wires*, J Phys Cond Mat 20, 045225 (2008)

**Other**
- Wang et al., *Excess-silver-induced bridge formation in a silver sulfide atomic switch*, APL 93, 152106 (2008)
Traditional quantum-based software packages can model either isolated molecules or periodic systems.

Gaussian, DMOL, TurboMol

Uniqueness of ATK

ATK is the only commercial software that can model complex nanostructures that combine molecules with periodic systems and macroscopic elements.

VASP, CASTEP, FLAPW, Wien2k
Main capabilities

- Spin-dependent electronic structure
  - Molecules (and supercells)
  - Periodic systems (crystals, nanowires, nanotubes)
  - Quasi-periodic systems (slabs)
- Spin-dependent quantum transport calculations in homo- or heterogeneous two-probe systems under finite bias
  - Transmission probability, conductance, I-V characteristics, transmission eigenstates, spin-torque transfer
- Qualitative simulation of electrostatic gate
- Reaction pathways & transition states via nudged elastic bands (NEB)
- Geometry optimization & MD
- Parallelized
  - Optimized for transport calculations
  - Linear scaling for transmission calculations
Virtual experiments

- Compute quantities that can be compared to experiments
  - Current-voltage characteristics
  - Co-linear spin torque transfer
  - Conductance
  - Bias-induced forces
  - Reaction pathways & activation energies
Analyzing quantum transport mechanisms

- ATK provides several analysis tools for understanding transport mechanisms
  - K-point resolved transmission
  - Transmission spectrum and surface DOS
  - Molecular projected self-consistent Hamiltonian eigenstates
  - Transmission eigenvalues and eigenchannels
Large-scale systems

- Nanowires, multiwall nanotubes and complex interface structures can easily contain several hundred atoms per unit cell.
- In order to treat effects from defects (including doping), very large unit cells are also required.
- ATK can handle very large systems (over 1,000 atoms).
Two-probe systems, electrodes

- A two-probe system consists of
  - left and right electrodes
  - a central scattering region
- Each electrode is a semi-infinite periodic system
  - Cleaved bulk crystal (e.g., a gold [111] surface)
  - Carbon nanotube, graphene, atomic chain, etc
- The two electrodes can be different
  - Two different metals
  - Two different carbon nanotubes
  - Metal-nanotube contact
  - Different spin-polarization (magnetic tunnel junctions)
The scattering region can be … anything!

- A molecule (e.g. between two metal surfaces)
- A piece of a carbon nanotube (e.g. a metal-nanotube-metal contact)
- A graphene nanoribbon zigzag/armchair contact
- A periodic structure (layered interfaces)
Interface boundary conditions

- Periodic boundary conditions are applied in the transverse plane
  - Makes it simple to model real interfaces, e.g. with surface impurities
  - Vacuum padding for 1D electrodes like nanotubes and wires
Transport boundary conditions

- Scattering boundary conditions apply in the transport direction
  - Electrons flow through the system under the influence of an applied voltage bias
  - Non-equilibrium electron distribution described by NEGF
  - Electric current is due to ballistic, coherent tunneling, computed using the Landauer formalism
Spintronics and magnetism

- In addition to the electronic current, ATK can compute the
  - spin current
  - spin torque transfer (STT)
  - tunnel magneto resistance (TMR)
Transistor simulations

- The ability of ATK to simulate an electrostatic gate enables calculations of transistor characteristics such as
  - Ambipolar characteristic
  - On-current
  - On/off current ratio
  - Leakage current
  - Sub-threshold swing

- Gate is introduced as a pure shift of the central Hamiltonian elements

B. Huang et al., APL 91, 253122 (2007)
Surface reactions and catalysis

Via an open source NEB (nudged elastic bands) module, ATK can compute reaction pathways and activation energies for catalytic reactions on surfaces.
Detailed list of features, Atomistix ToolKit

- **Electronic structure calculations**
  - SIESTA-based method, plus inclusion of indirect atom pairs for improved accuracy
  - Up to double-zeta double polarized (DZDP) numerical atomic orbital basis sets, with detailed user control of basis set parameters
  - Norm-conserving (Troullier-Martins) pseudopotentials provided for all elements, with possibility to use customized pseudopotentials
  - LDA-PZ, GGA-PBE GGA-revPBE exchange correlation potentials (also spin-polarized)
  - Fermi level smearing for improved convergence stability
  - Customizable Broyden/Pulay mixing for self-consistent scheme
  - Monkhorst-Pack k-point sampling grids

- **Calculation of**
  - Molecular spectra
  - Band structure of periodic structures
  - Eigenfunctions (molecular orbitals, Bloch functions)
  - Mulliken population analysis
  - Real-space electron density and effective potential
  - Forces (analytic Hellmann-Feynman)

- **Ion dynamics**
  - Quasi-Newton or steepest descent method
  - Constraints: fixed positions
  - Nudged Elastic Band (NEB) transition state analysis

- **Transport calculations**
  - Two-probe systems NEGF using the TranSIESTA method (self-energy coupling to semi-infinite leads)
  - Green's function description of non-equilibrium electron distribution in scattering region
  - Finite bias
  - Ability to treat heterogeneous systems through multi-grid solution to Poisson's equation
  - Simulation of electrostatic gate

- **Transport analysis**
  - Transmission coefficients (k-point resolved) and transmission spectrum
  - Spin-dependent current and conductance/resistance
  - Transmission eigenvalues and real-space eigenchannels
  - Surface density of states
  - Real-space local density of states
  - Fast evaluation of linear response current
  - Collinear spin-torque transfer
  - Molecular Projected Self-Consistent Hamiltonian eigenvalues and real-space eigenfunctions

- **Work-flow control**
  - Store and restore the state of a calculation for deferred analysis, restart, or initialization of a new calculation via the self-consistent density matrix
NanoLanguage

- Fully programmable object-oriented Python scripting interface to ATK
  - Transparent - the Python syntax is simple yet powerful, with good structural overview
  - Modularized
  - Extendable - integrate your own or third-party algorithms with ATK

- Tying the platform together
  - Integrated with the GUI, Virtual NanoLab
  - Wrapping of third-party codes

- Interpreted language
  - Can be used interactively
  - Comes with “batteries included” (scientific modules)
  - Cross-platform compatible scripts
  - All performance-critical parts of ATK are written in C++/Fortran

- Online user Forum for tips, tricks, script resources, etc
NanoLanguage offers

- **Control of parameters**
  - Loop over numerical parameters
  - Set up parameterized geometries

- **Control of flow**
  - Automatically converge in accuracy parameters
  - Decision-making scripts

- **Access to data in native Python format**
  - Customized analysis
  - Export data in any desired format

- **Extendability**
  - Implement new algorithms, backed by ATK
  - Wrap other software packages
  - Anything you otherwise can do in Python, applied to quantum chemistry!
- Interactive builders for
  - Molecules
  - Crystals
  - Nanotubes
  - Two-probe systems (general and specialized, like MTJs)
- 3D visualization of structures and results
  - Electron density, potentials, etc, as isosurfaces or contour plots
  - Superimpose plots on geometry
  - Export plots as images in common formats
- Interactive generation and export of NanoLanguage scripts
  - Structures and geometries
  - Calculations and analysis
- Internal NanoLanguage interpreter
  - Import user-defined geometry scripts for visualization or calculation setup
  - Built-in script editor
- Local execution of NanoLanguage scripts via drag-and-drop
Build complex molecules with a few mouse-clicks with the **Molecular Builder**
  » Bond angles and lengths are automatically adjusted according to specified hybridization and bond order
  » Fine-tune the geometry manually
  » Hydrogen added automatically
  » Attach pre-built side-groups from the **Crystal Cupboard**

**Calculate and plot molecular spectra**

**Visualize molecular wave functions and electron densities in the **Nanoscope**
Crystals

- Browse the **Crystal Cupboard** for over 500 pre-built crystal templates
- Build your own crystal from scratch in the **Bulk Builder**
  - Create slab models
  - Make supercells & slab models
- Calculate and plot the spin-dependent band structure
- Visualize Bloch states
**Nanotubes & Graphene**

- Build nanotubes (C, Si, Au, ...) in the **Nanotube Grower** with a few clicks
- Use scripting coupled with the GUI to set up
  - boron-nitride nanotubes
  - graphene nanoribbons
- Introduce defects or ad-atoms and study the influence on the band structure
- Create nanotube or graphene two-probe systems to study current/voltage characteristics, spin-polarized transport, etc
Two-probe systems

- Build two-probe systems easily in the Atomic Manipulator
  - Cleave any crystal by specifying the Miller indices and surface cell
  - Align and rotate entire molecules in the scattering region
  - Control over individual atom positions, delete/add atoms
- Also support for 1D electrodes
  - Study transport properties of functionalized nanotubes, etc
Magnetic Tunnel Junction Builder

- Instantly generate advanced MTJ two-probe geometries
- Support for any FeCo type materials (bcc [100] surfaces)
- Detailed control over all layer separations
- Buckling
- Fine-tune or introduce defects in the Atomic Manipulator
NanoLanguage in VNL

- VNL is designed to help the user learn and master NanoLanguage
- Builders generate atomic geometries represented as NanoLanguage scripts
  - Drag-and-drop to other instruments in VNL
  - Drag-and-drop to editor (internal or external) for direct editing
  - Use generated scripts as templates for advanced geometries
- Verify and troubleshoot custom code
  - Define custom geometries externally in script, then drop code directly on Nanoscope for visualization
- Drop scripts on **Job Manager** to execute script in ATK
  - Runs in dedicated thread for optimal performance
  - Restricted to local host
- Drop geometry on **NanoLanguage Scripter** to set up the calculation
  - See next slide!
NanoLanguage Scripter

- Use the **NanoLanguage Scripter** to generate complete calculation scripts, ready for running, in just a few steps.
- **Supports**
  - All ATK keywords, including I/O
  - All analysis options
  - Geometry optimization
- **Exports nicely formatted scripts, ready-to-run even in parallel**
  - Use generated scripts as templates for more advanced coding.
Performance

- State-of-the-art parallel DFT code
  - MPI parallelization for k-points and energy points
  - OpenMP for threading on multi-core CPUs
  - Optimized code & libraries provide excellent performance and scaling

- Examples:
  - MgO bulk supercell with 1,024 atoms converges in 16 hours on a single node, using 3 Gb memory (DZP basis set)
  - Au/Si/Au two-probe with 1,166 atoms, 24 hours on 10 nodes, 2 Gb (SZ basis set)
## Parallel scaling

- Supercluster test, ATK 2008.10
- Self-consistent calculation scales well up to 32 nodes
- Almost linear scaling for transmission/current calculations up to >100 nodes

### Test system

<table>
<thead>
<tr>
<th>System</th>
<th>TSUBAME grid cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td>Computer</td>
<td>Sun Fire X4600 with Infiniband interconnects</td>
</tr>
<tr>
<td>CPU</td>
<td>Dual-core AMD Opteran 880 @ 2.4GHz, 8 CPUs (16 cores) + 32 Gb RAM / node</td>
</tr>
<tr>
<td>OS</td>
<td>SUSE Linux Enterprise Server 9 SP 3</td>
</tr>
</tbody>
</table>

### Model

- **Model:** Si nanowire between Au surfaces

<table>
<thead>
<tr>
<th>Model</th>
<th>Electrodes: Au(100)</th>
<th>Molecule: Si nanowire</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basis set</td>
<td>DoubleZetaPolarized</td>
<td></td>
</tr>
<tr>
<td>Exchange-correlation</td>
<td>LDA-PZ</td>
<td></td>
</tr>
<tr>
<td>Mesh cut-off</td>
<td>150 Ry</td>
<td></td>
</tr>
<tr>
<td>k-point sampling (SCF)</td>
<td>(5, 5, 500)</td>
<td></td>
</tr>
<tr>
<td>k-point sampling (DOS, Transmission)</td>
<td>(10, 10)</td>
<td></td>
</tr>
</tbody>
</table>
## Parallel scaling, detailed results

**Table: Calculation time and speed-up**

<table>
<thead>
<tr>
<th>CPU cores</th>
<th>Calculation time</th>
<th>Speed-up</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SCF</td>
<td>Physical properties</td>
<td>Total</td>
</tr>
<tr>
<td>1</td>
<td>67h52m</td>
<td>106h51m</td>
<td>174h43m</td>
</tr>
<tr>
<td>4</td>
<td>19h27m</td>
<td>27h29m</td>
<td>46h56m</td>
</tr>
<tr>
<td>8</td>
<td>8h24m</td>
<td>14h32m</td>
<td>22h56m</td>
</tr>
<tr>
<td>16</td>
<td>6h19m</td>
<td>7h50m</td>
<td>14h09m</td>
</tr>
<tr>
<td>32</td>
<td>4h37m</td>
<td>3h55m</td>
<td>8h32m</td>
</tr>
<tr>
<td>64</td>
<td>4h00m</td>
<td>1h59m</td>
<td>5h59m</td>
</tr>
<tr>
<td>128</td>
<td>3h37m</td>
<td>1h04m</td>
<td>4h41m</td>
</tr>
</tbody>
</table>

**Graph: Speed-up vs. CPU Cores**

- **SCF**: Linear speed-up
- **Analysis**: Non-linear speed-up
- **Total**: Combined SCF and Analysis time
- **Linear**: Ideal linear speed-up

**Inset Graph:**

*Total time = SCF + Analysis*
Supported platforms

- Atomistix ToolKit
  - Linux
    - 32-bit version, optimized for i686
    - 64-bit version, optimized for x86_64
    - Parallelized using MPICH2 (statically linked)
  - Windows
    - 32-bit version for XP, Vista, 2000

- Virtual NanoLab
  - 32-bit version for Linux/Windows i686
  - Also runs on x86_64

- FLEXlm license manager
  - Node-locked or floating licenses

BEST CHOICE FOR HIGH PERFORMANCE

ATK and VNL run on most Linux distributions, with official support for
- RedHat Enterprise Linux (4.x, 5.x)
- SUSE Linux Enterprise (9.x, 10.x)
Want to learn more?
Please visit our website
http://www.quantumwise.com
to download a FREE trial version