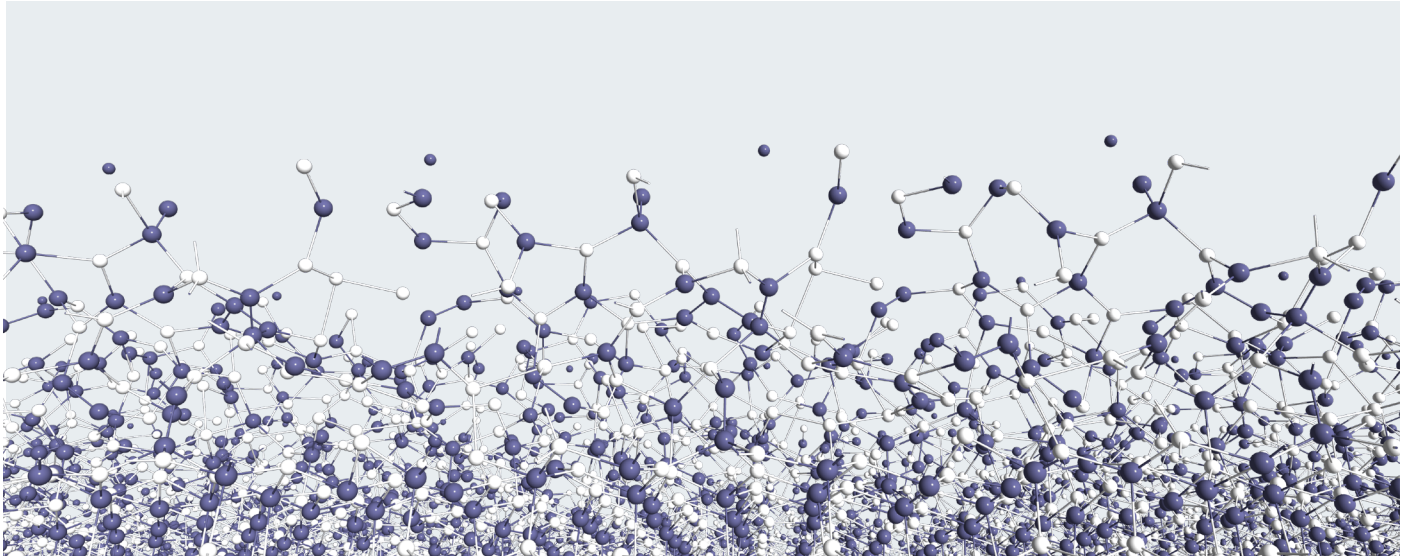
SYNOPSYS®

QuantumATK Release Features

Last amended: June 2020

QuantumATK R-2020.09

QuantumATK 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. QuantumATK combines the power of a Python scripting engine with the ease-of-use provided by an intuitive graphical user interface, NanoLab. All simulation engines share a common infrastructure for analysis, ion dynamics and parallel performance techniques.



Downloading and Installing QuantumATK R-2020.09

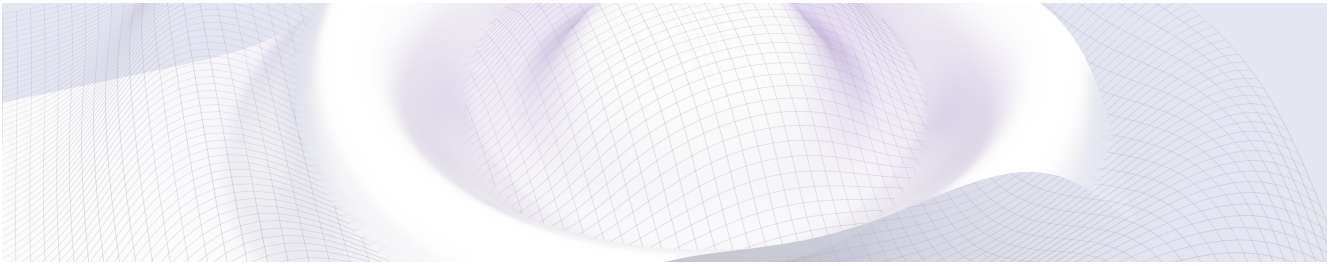
Download

If you are a customer entitled to maintenance services, you can access QuantumATK Q-2019.12 and download installation notes directly from **SolvNetPlus:** https://solvnetplus.synopsys.com.

License

To run QuantumATK R-2020.09, customer must use the Synopsys Common Licensing (SCL) software, version 2018.06-SP1 or later. License key files and the latest version of SCL can be downloaded from your account on SolvNetPlus.

> If you are not a current customer and you wish to try out QuantumATK, please apply for a free 30-day evaluation license on the Synopsys **EVAL portal:** https://eval.synopsys.com/



New Features in QuantumATK R-2020.09

DFT & Analysis Objects Updates

- Hybrid-functional method (HSE) for LCAO, which enables accurate DFT simulations of large-scale systems with modest computational resources. Up to 100x faster than plane-wave HSE for smaller systems, and tested on as many as 2,000 atoms.
- 3D-corrected k·p method to speed-up band structure and DOS calculations with plane-wave HSE from days/hours to less than a minute.
- Shell DFT+1/2 method for more accurate semiconductor band gaps.
- Nuclear magnetic resonance (NMR) simulations of molecules and solids, including advanced analysis of calculated NMR shielding tensors and chemical shifts in GUI.

Dynamics Updates

- Improved methods to quickly obtain geometry estimates of a structure using classical force fields.
- Newly added universal force field (UFF) covering the entire periodic table and thus allowing a wide range of materials to be simulated.
- Device geometry optimization improvements, resulting in better optimized device configurations.
- Nudged elastic band simulation improvements, including added possibility to use more flexible constraints.

Polymer Simulation

- Crosslinking reaction tool for building thermoset polymers, which form cross-linked or 3D network structures, such as epoxy/amine systems, as well as rubber-like network structures.
- Added support for united atoms and coarse-grained polymers to significantly accelerate simulations.
- New option to create your own monomers, add monomers in existing forward and now reverse orientations, in addition to using a convenient plug-in for assigning monomer tags to define monomer linking reactions.
- New user-friendly polymer analysis tools, which can be employed to plot end-to-end distances, free volume, polymer segments, molecular order parameters, and radius of gyration.

Performance Improvements

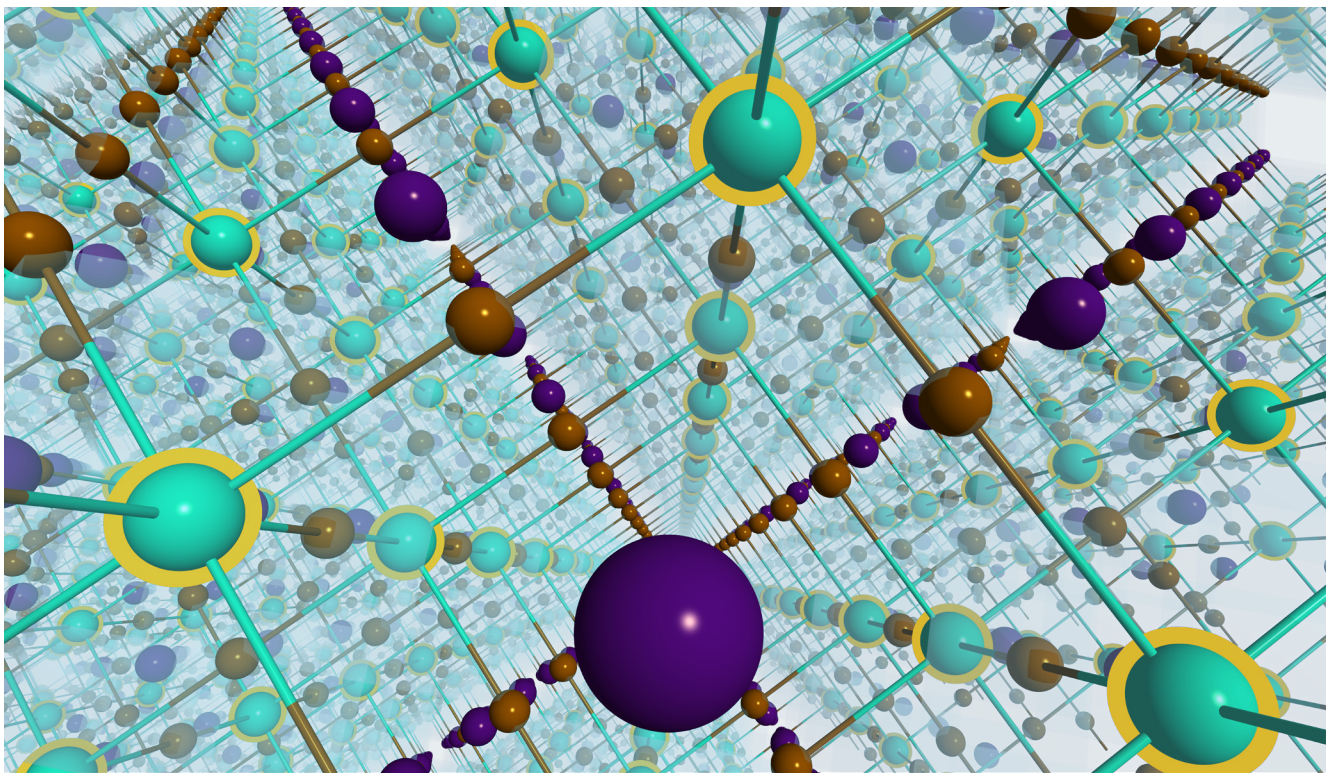
- 2x faster ab initio molecular dynamics simulations.
- Enhanced parallel performance of dynamical matrix and Hamiltonian derivatives.
- Significant speed-ups and reduced memory consumption of parallel DFT-PlaneWave simulations
- 30-60% speed-up for the SCF loop for DFT-LCAO and semi-empirical simulations.
- Improved serial and parallel performance of zero-bias NEGF calculations of symmetric and asymmetric device geometries.
- 6x speed-up and 50% reduced memory usage of projected local density of states (PLDOS) simulations.

NanoLab GUI Updates

- State-of-the-art new molecular builder, enabling bond lengths and angles editing, as well as a new bonds plug-in for finding, adding, or deleting static bonds in various configurations.
- Improved tool for generating good starting interface geometries, which is particularly useful when scanning across multiple interfaces.
- Other builder improvements, including enhanced GUI and added scripting builder functions to create devices, and improved Packmol builder for creating amorphous configurations.
- Enhanced 2D plotting framework to further tailor your plots, and an exposed plot framework API to build your own custom plots using scripts.
- User-friendly framework for setting up, submitting, and analyzing large number of simulations for more efficient high-throughput material screening.

Sentaurus Materials Workbench Updates

- Surface process module for setting up and running flexible simulation protocols of deposition, etching and sputtering.
- Plug-in for conveniently adsorbing molecules on a surface.
- New and improved features for defect simulations, including a new band gap correction method for defect trap levels, which gives more accurate results and can speed-up calculations by 75x, and the possibility to use multiple charge states in transition path list calculations.
- Easy setup and analysis of a large set of different grain boundaries, as well as user-friendly script generation for linking simulation outputs to TCAD Raphael FX for interconnect simulations.



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