QDFT

HIGH PERFORMANCE DFT USING TRADITIONAL GAUSSIAN BASIS SETS FOR THE 21ST CENTURY'S COMPUTATIONAL DRUG DESIGNS, FORCE FIELDS AND AI DEVELOPMENTS

- New QFC method for linear scaling Coulomb solution
- New QFX method with advanced DFT atomic grid technology
- Modern and extremely efficient C++ implementation
- Same accuracy as traditional all electron DFT programs
- Implementation of Grimme’s D4 dispersion corrections
- Improved D4 accuracy via new fitting scheme for basis set-functional pairs
- Extraordinary speed on ordinary CPUs and by keeping full double precision accuracy

QUICK POINTS

- Extremely fast DFT energy and force calculations with accurate basis sets and XC numerical grids
- Implementation of Grimme's D4 dispersion corrections
- More accurate D4 dispersion corrections for practical basis sets by optimizing parameters for functional-basis set pairs (see VDW-D4-Remarks.pdf for details)
- Support of using external fields via point charges
- Geometry optimizations including options to freeze atoms, bonds, angles, torsion angles
- Continuum solvation model via semiempirical QM
- Native Linux version as well as docker image
- Convenient and fair usage based licensing scheme
- Molecular Dipoles
- Atomic distributed multipoles
- EEQ Charges

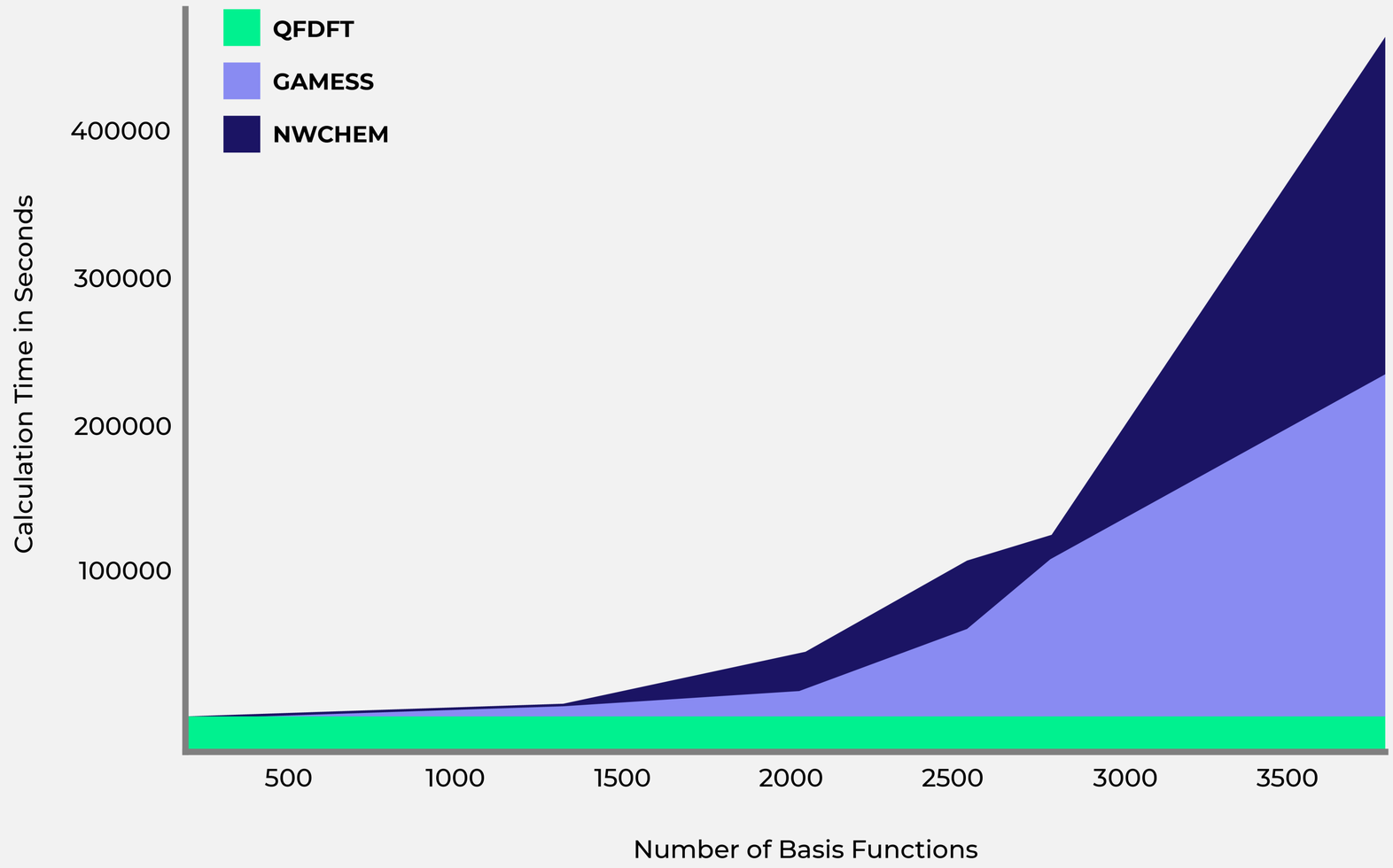
BETA FEATURES

- Charge density, electrostatic potentials, HOMO, LUMO etc.
  on cube-like grids for visualizations
- Maybe other atomic properties
- Maybe vibrations and thermodynamic properties

For more information, please take a look at our release notes

COMING SOON

Comparative Study Visual



COMPARE

Our commercial DFT code with license fee is cheaper than using free software!

If you use freely available quantum chemistry code like NWCHEM, GAMESS US or PSI4 then take a look at this realistic cost analysis using real word examples!

Cost comparisons of a month-long ab initio DFT project using QFDFT with assumptions of:

1. Buying a capable Intel Xeon based node with 64 physical cores for $12,000 and using it for 5 years
2. The electricity usage is about 600W with an additional 600W for cooling
3. The electricity cost in the USA is about $0.12/kWh and about $0.39/kWh in Germany (DE in the table below)
4. The QFDFT code is 20 times faster than those free programs (This is a very conservative assumption)
5. We have a facility for the computers and hardware and software maintenance is done for free

	Using Free DFT Code	Using QFDFT
Hardware Cost/month	~$200	~$200
Electricity Cost/month	~$100 (US), ~$350 (DE)	~$100 (US), ~$350 (DE)
License Fee/month	$0	~$700
Total Cost/month	~$300 (US), ~$550 (DE)	~$1,000 (US), ~$1,250 (DE)
Total Project Cost	**$6,000 (US), $11,000 (DE)**	**$1,000 (US), $1,250 (DE)**
Results After	**20 months**	**1 month**

VALUE

Cost comparisons of a month-long ab initio DFT project with QFDFT with assumptions of:

1. Renting a capable Intel Xeon based node with 64 physical cores for $5/hour on Amazon EC2

2. The QFDFT code is 20 times faster than those free programs (This is a very conservative assumption)

3. No need for computer rooms and no need for any hardware and software maintenace

	Using Free DFT Code	Using QFDFT
On-Demand Cost/month	~$3,600	~$3,600
License Fee/month	$0	~$700
Total Cost/month	~$3,600	~$4,300
Total Project Cost	**$72,000**	**$4,300**

VALUE (cont.)

DFT-D4, def2-TZVP, rev-TPSS energies, 52 cores

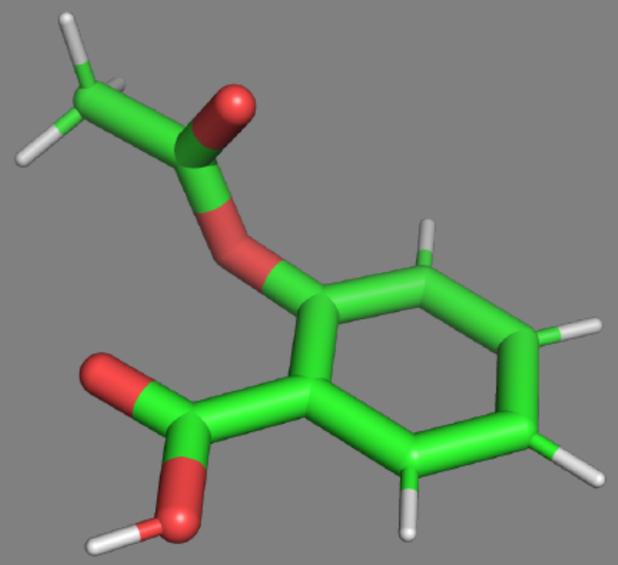
Energy	12 seconds
QM semiempirical optimization + Energy	14 seconds
QM semiempirical opt + DFT-D4 opt + Energy	110 seconds

Comparative Study

Energy Calculations			Gradients	
QFTDFT	GAMESS	NWCHEM	QFTDFT	GAMESS
17	129	240	3	27

(Timings in seconds on an 18-core Intel i9, DFT, dev2-SVPD, TPSS)

ASPIRIN 19 atoms
(WELL KNOWN MEDICATION)



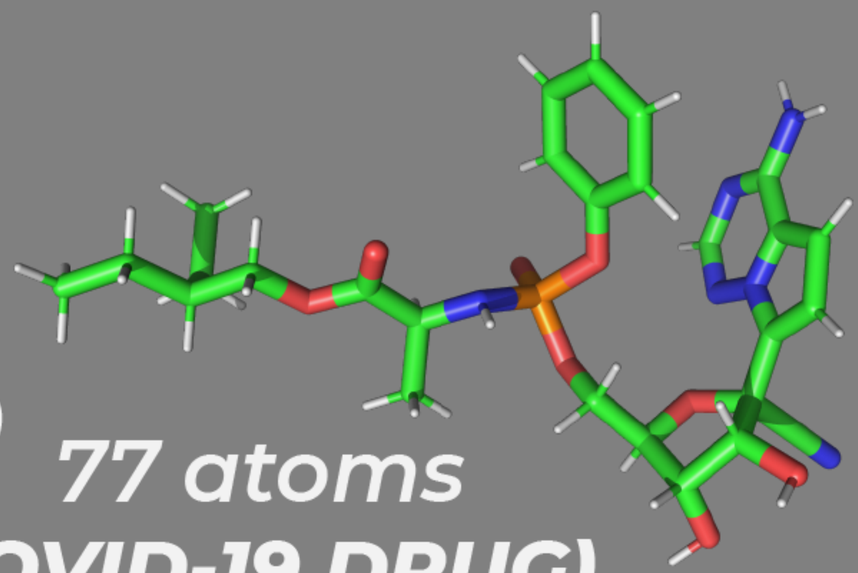
DFT-D4, def2-TZVP, rev-TPSS energies, 52 cores

Energy	87 seconds
QM semiempirical optimization + Energy	94 seconds
QM semiempirical opt + DFT-D4 opt + Energy	1,438 seconds

Comparative Study

Energy Calculations			Gradients	
QFTDFT	GAMESS	NWCHEM	QFTDFT	GAMESS
131	7,213	6,534	26	1,104

(Timings in seconds on an 18-core Intel i9, DFT, dev2-SVPD, TPSS)



REMDESIVIR 77 atoms
(ANTIVIRAL MEDICATION, COVID-19 DRUG)

DFT-D4, def2-TZVP, rev-TPSS energies, 52 cores

Energy	189 seconds
QM semiempirical optimization + Energy	244 seconds
QM semiempirical opt + DFT-D4 opt + Energy	2,502 seconds

Comparative Study

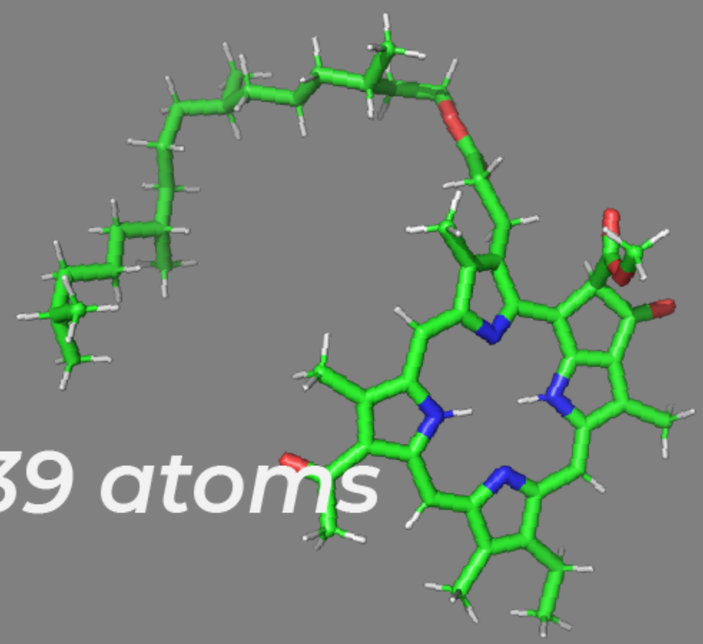
Energy Calculations			Gradients	
QFTDFT	GAMESS	NWCHEM	QFTDFT	GAMESS
272	18,588	42,673	50	5,044

(Timings in seconds on an 18-core Intel i9, DFT, dev2-SVPD, TPSS)

BACTERIO-PHEOPHYTIN

(ROLE IN ELECTRON TRANSFER)

139 atoms



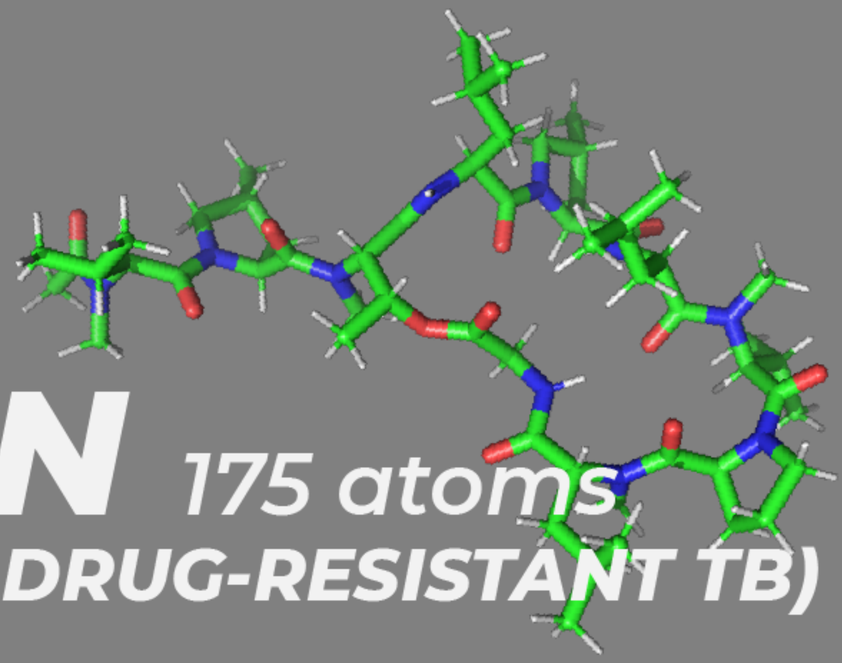
DFT-D4, def2-TZVP, rev-TPSS energies, 52 cores

Energy	310 seconds
QM semiempirical optimization + Energy	356 seconds
QM semiempirical opt + DFT-D4 opt + Energy	3,425 seconds

Comparative Study

Energy Calculations			Gradients	
QFTDFT	GAMESS	NWCHEM	QFTDFT	GAMESS
526	61,490	104,402	113	9,924

(Timings in seconds on an 18-core Intel i9, DFT, dev2-SVPD, TPSS)



GRISELIMYCIN *175 atoms*
(PROMISING LEAD IN TREATING DRUG-RESISTANT TB)

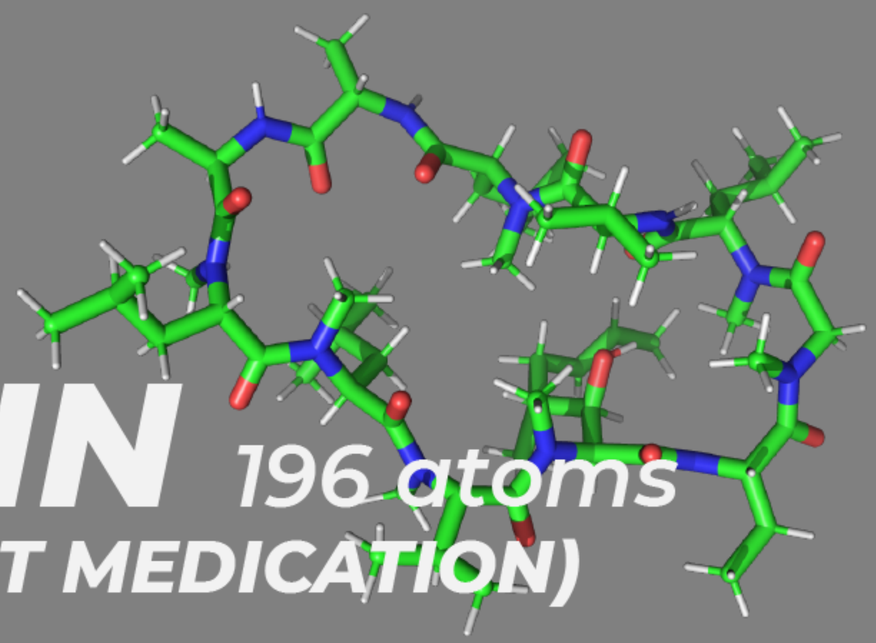
DFT-D4, def2-TZVP, rev-TPSS energies, 52 cores

Energy	385 seconds
QM semiempirical optimization + Energy	432 seconds
QM semiempirical opt + DFT-D4 opt + Energy	5,544 seconds

Comparative Study

Energy Calculations			Gradients	
QFTDFT	GAMESS	NWCHEM	QFTDFT	GAMESS
805	109,263	120,779	163	13,792

(Timings in seconds on an 18-core Intel i9, DFT, dev2-SVPD, TPSS)



CYCLOSPORIN 196 atoms
(USED AS IMMUNOSUPRESSANT MEDICATION)

DFT-D4, def2-TZVP, rev-TPSS energies, 52 cores

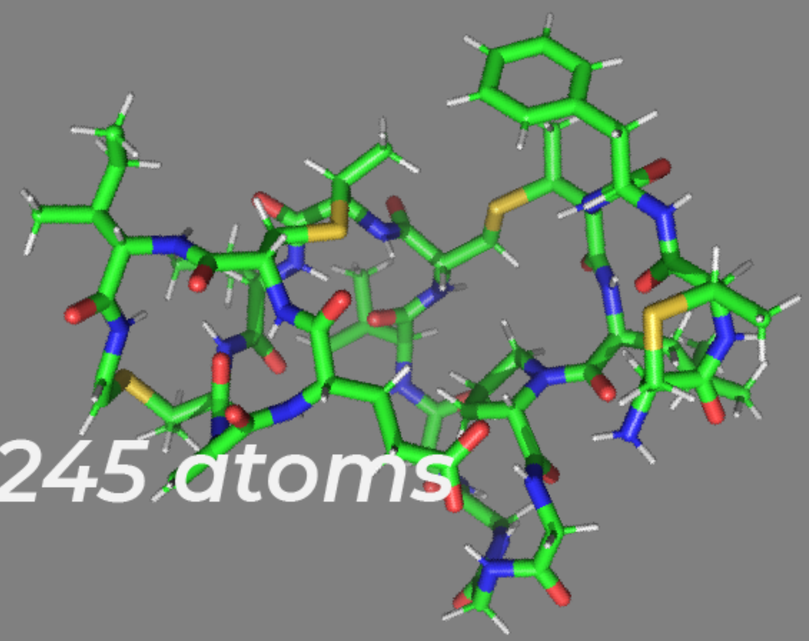
Energy	705 seconds
QM semiempirical optimization + Energy	987 seconds
QM semiempirical opt + DFT-D4 opt + Energy	5,975 seconds

Comparative Study

Energy Calculations			Gradients	
QFTDFT	GAMESS	NWCHEM	QFTDFT	GAMESS
1,025	232,893	461,391	243	31586

(Timings in seconds on an 18-core Intel i9, DFT, dev2-SVPD, TPSS)

MERSADICIN
(ANTBIOTIC)



245 atoms