Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Linear algebra in *ab initio* computational chemistry

Evgeny Epifanovsky

September 18, 2018

Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Atomistic simulations in chemistry:

- Molecular mechanics methods
  (structure and properties of large molecules)
- Plane-wave electronic structure methods
  (periodic infinite systems, e.g. crystals)
- Gaussian-basis electronic structure methods
  (finite molecular structures)

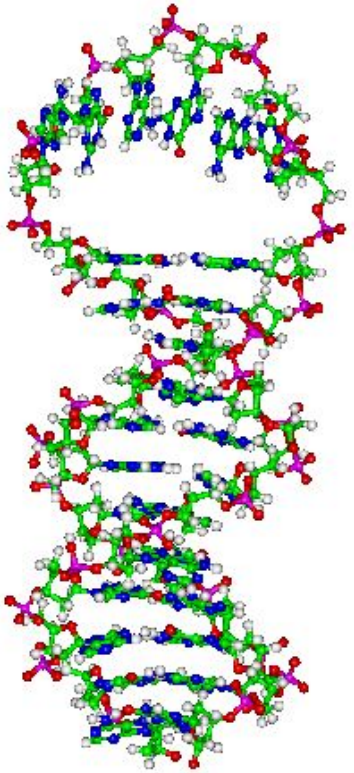

Image: Dr. Michal Sabat, Molecular Structure Laboratory, Department of Chemistry, University of Virginia

What is Q-Chem?

Established in 1993, first release in 1997.

Commercially supported software

Q-Chem 3.0 (2006)
4.0 (2012)
4.1 (2013) 4.2 (2014)
4.3 (2015) 4.4 (2016)
5.0 (2017)
5.1 (2018)

Development platform

Supported infrastructure for
state-of-the-art quantum chemistry

Open source for developers

> 200 contributors (Q-Chem 5)

Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Computational kernels prevalent in typical quantum chemistry simulations

		Other	MV	MM	Tensor	Examples
DFT	Coulomb	100%				$J_{ij} = V_{ijkl} P_{kl}$
	DF Coulomb	70%	30%			$M_{pq} \quad X_q = V_{ijp} P_{ij} M_{pq} \quad J_{ij} = X_q V_{ijq}$
	Exchange	90%			10%	$K_{ik} = V_{ijkl} P_{jl}$
	DF Exchange	10%		90%		$K_{ik} = B_{ijp} B_{kjp}$
	XC	50%		50%		$P_i = D_{mn} X_{mi} X_{ni} \quad G_{mn} = F_i X_{mi} X_{ni}$
RI-MP2		10%		90%		$T_{ijab} = B_{iap} B_{jbp} - B_{ibp} B_{jap}$
CCSD(T)		40%			60%	$T_{ijkabc} = V_{kdab} Z_{ijcd}$