Q-CHEM

A QUANTUM LEAP INTO THE FUTURE OF CHEMISTRY

What is new in Q-CHEM 5

Q-Chem User Workshop, Munich

August 26, 2017

New Density functionals

- **Combinatorially designed functionals:**
  B97M-V, ωB97X-V, ωB97M-V (Mardirossian and Head-Gordon)
- **Constraint-based density functionals:**
  SCAN family, MS1, MS2 (Perdew and co-workers)
- **Latest Minnesota functionals:**
  MN15, MN15-L, *revM06-L*
- **Full range of dispersion corrections:**
  - VdW functionals
  - D3 corrections with choice of damping
- **All other significant functionals:** more than 200 to choose from

Implementation of exchange-correlation density functionals in Q-CHEM by Dr. Narbe Mardirossian.

New density functionals

Functional	NCED	NCEC	NCD	IE	ID	TCE	TCD	BH	EBL	EBE
SPW92	2.14	37.77	7.60	2.22	6.76	42.23	65.35	19.55	0.195	2.81
PBE	1.96	4.08	3.26	1.15	6.53	9.22	15.58	9.17	0.327	2.16
TPSS	2.58	8.90	2.63	1.39	8.44	5.94	10.45	8.03	0.398	2.80
B3LYP	2.86	8.91	1.77	1.49	11.10	5.24	11.97	5.96	0.643	3.04
PBE-D3(BJ)	0.46	5.78	3.67	0.71	5.19	9.67	17.20	9.99	0.049	0.42
revPBE-D3(BJ)	0.49	6.60	2.54	0.77	5.21	6.60	9.91	8.30	0.053	0.44
BLYP-D3(BJ)	0.34	2.18	2.82	0.68	11.40	6.63	11.11	9.91	0.031	0.25
B97-D3(BJ)	0.47	4.82	2.52	0.78	9.15	4.66	7.92	8.32	0.045	0.42
TPSS-D3(BJ)	0.38	2.28	3.06	0.69	6.47	5.88	8.86	8.72	0.070	0.33
SCAN-D3(BJ)	0.54	9.18	3.41	0.55	4.46	5.25	6.39	7.83	0.037	0.60
M06-L	0.55	2.20	1.87	0.71	10.16	5.44	12.97	6.85	0.043	0.60
B97M-rV	0.22	0.67	2.04	0.28	6.45	3.57	4.78	4.36	0.025	0.17
PBE0-D3(BJ)	0.44	4.45	2.28	0.58	3.47	4.76	8.72	4.91	0.043	0.46
B3LYP-D3(BJ)	0.31	3.02	1.88	0.49	8.51	3.72	5.97	5.65	0.022	0.37
ωB97X-D	0.37	1.01	1.46	0.67	3.11	3.44	5.79	2.34	0.038	0.42
ωB97X-V	0.24	0.64	1.23	0.27	2.72	3.41	5.01	2.44	0.042	0.15
TPSSh-D3(BJ)	0.36	1.73	2.49	0.62	5.29	5.55	5.92	6.63	0.068	0.33
M06-2X	0.43	2.52	0.99	0.50	5.56	3.29	7.23	2.57	0.077	0.33
MN15	0.47	1.83	0.96	0.71	4.06	3.76	6.44	1.98	0.042	0.60
ωB97M-V	0.18	0.48	1.13	0.28	2.05	2.48	4.30	1.68	0.014	0.15
Minimum	**0.18**	**0.48**	**0.91**	**0.27**	**2.05**	**2.48**	**4.30**	**1.68**	**0.014**	**0.15**
Best	**ωB97M-V**	**ωB97M-V**	**M08-SO**	**B97M-V**	**ωB97M-V**	**ωB97M-V**	**ωB97M-V**	**ωB97M-V**	**ωB97M-V**	**ωB97X-V**

From N. Mardirossian and M. Head-Gordon, *Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals*, Mol. Phys., 2017.

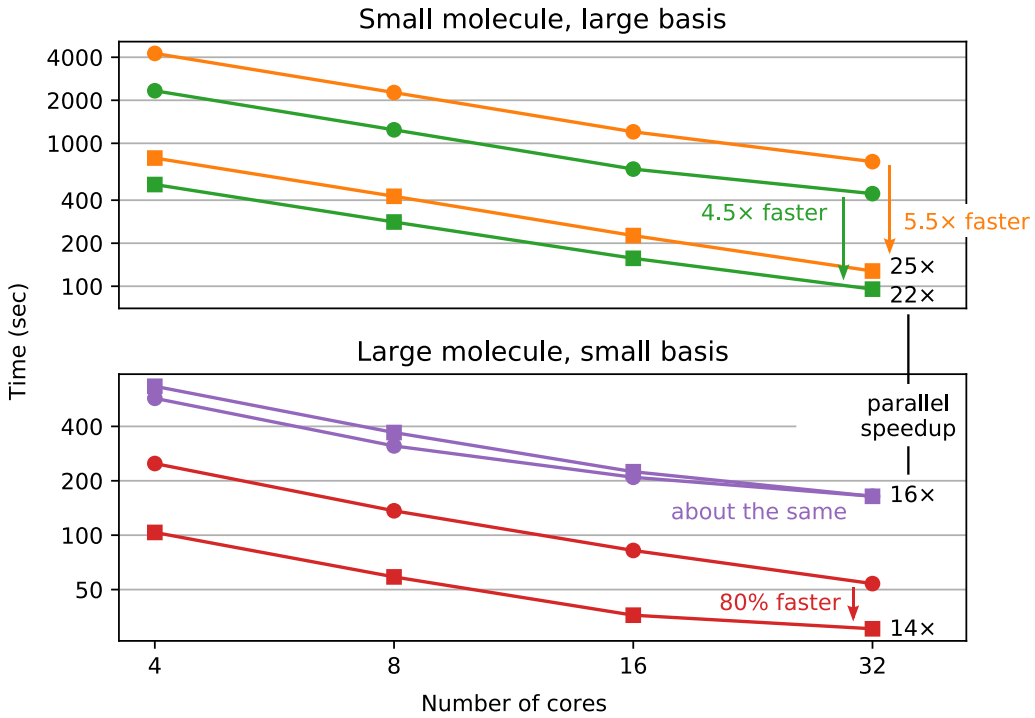
Other DFT improvements

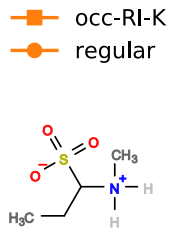
- **New standard integration grids:**

Grid	Parent	Default for
SG-2	(75, 302)	Mega-GGAs, B95- and B97-based functionals
SG-3	(99, 590)	Minnesota functionals

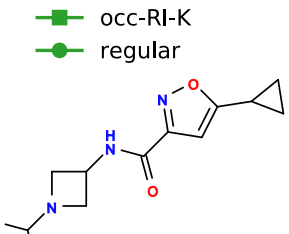
- **New forms of DFT-D3 dispersion correction:**
  DFT-D3(0), DFT-D3(BJ), DFT-D3(CSO), DFT-D3M(0), DFT-D3M(BJ), DFT-D3(op)
- **More efficient propagator algorithms for real-time TDDFT**

occ-RI-K algorithm

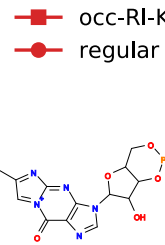




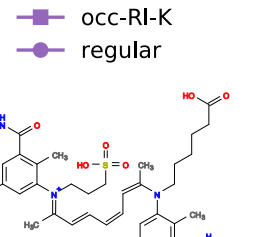
def2-QZVPPD
955 BSFs



def2-TZVPPD
995 BSFs



def2-SVP
513 BSFs



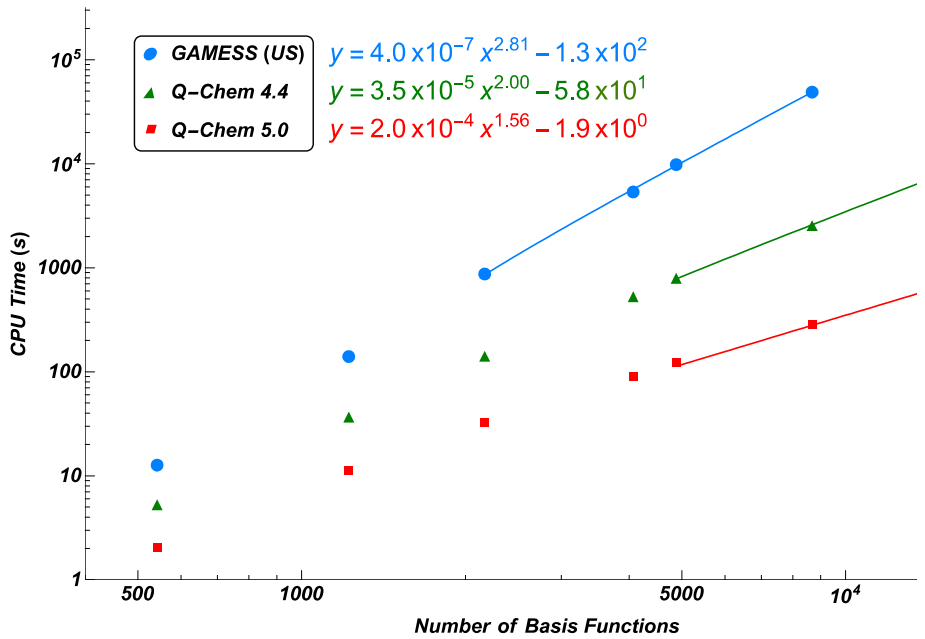
VDZ basis
843 BSFs

Implementation by Evgeny Epifanovsky, Joonho Lee, Fazle Rob, Samuel Manzer.

New ECP capabilities

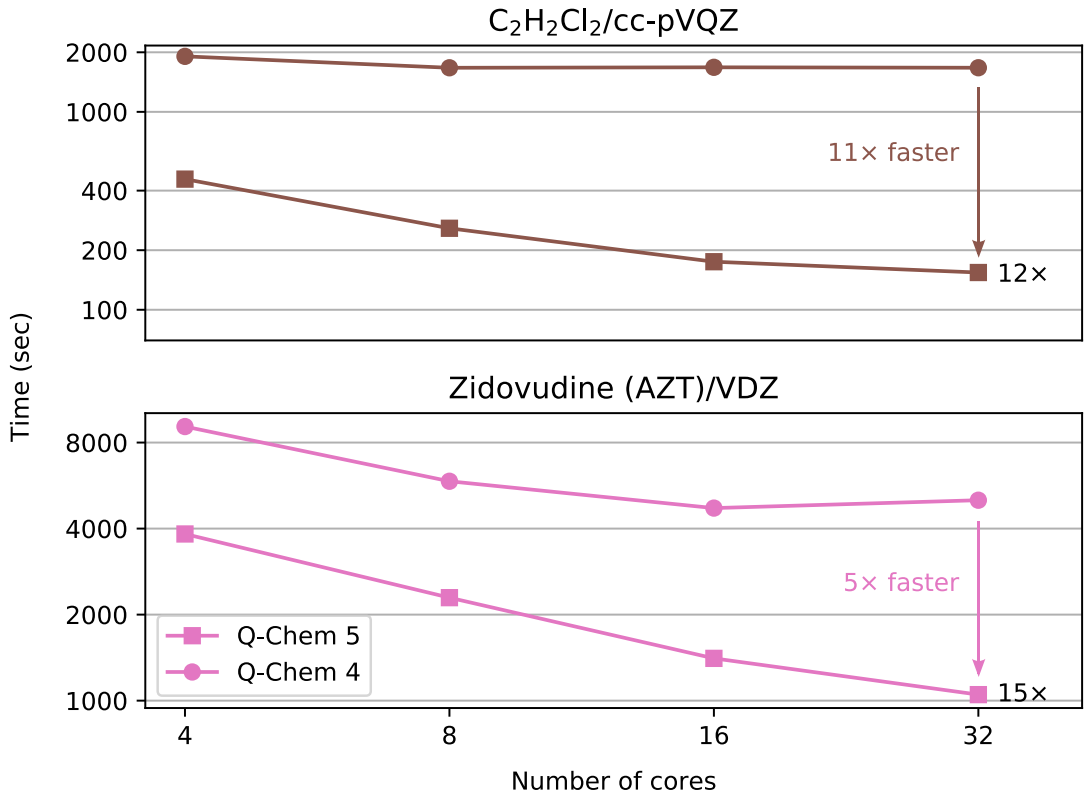
- No limit in basis function or projector angular momentum
- Stuttgart, Karlsruhe ECPs supported natively
- LANL2DZ, CRENBL/CRENBS, SBKJC ECPs supported through reconstruction
- Energy, analytic gradients and Hessians (5.1)

Implementation by Simon McKenzie.



Coupled-cluster methods

Improved parallel performance of CCSD(T) computations



Using *libxm*, *libpt* developed by Dr. Ilya Kaliman.

More info

- Poster at WATOC-2017 **PO3-248** on Thursday, August 31
- www.q-chem.com:
  - Q-CHEM User's Manual
  - Recorded webinar presentations
  - Teaching materials
  - Evaluation license request