



DFT Made Faster and More Accurate

Holger Dachsel, Prakashan Korambath,
Shawn Brown, Yihan Shao, Laszlo Fusti-Molnar,
Emil Proynov, Zhengting Gan, Nick Russ, Jing Kong

Q-Chem Inc.
Pittsburgh, PA

Parallel & GPU
HF&DFT

DFT Algorithms
FTC, mrXC, PBC

QM/MM, QM/QM
Yin-Yang

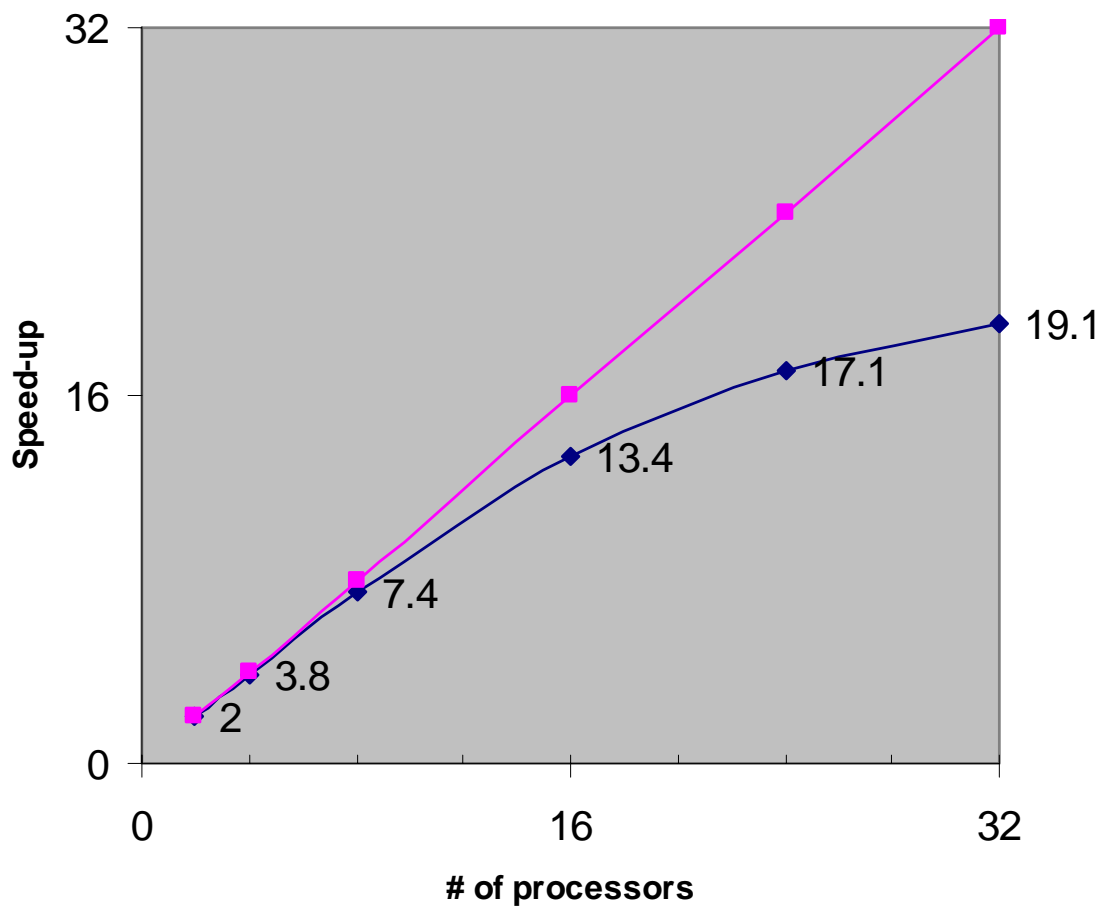
Functionals
PK06, XDM, RSC

Developers: *Dachsel, Korambath, Brown, Fusti-Molnar*

“qchem -np nproc input output”

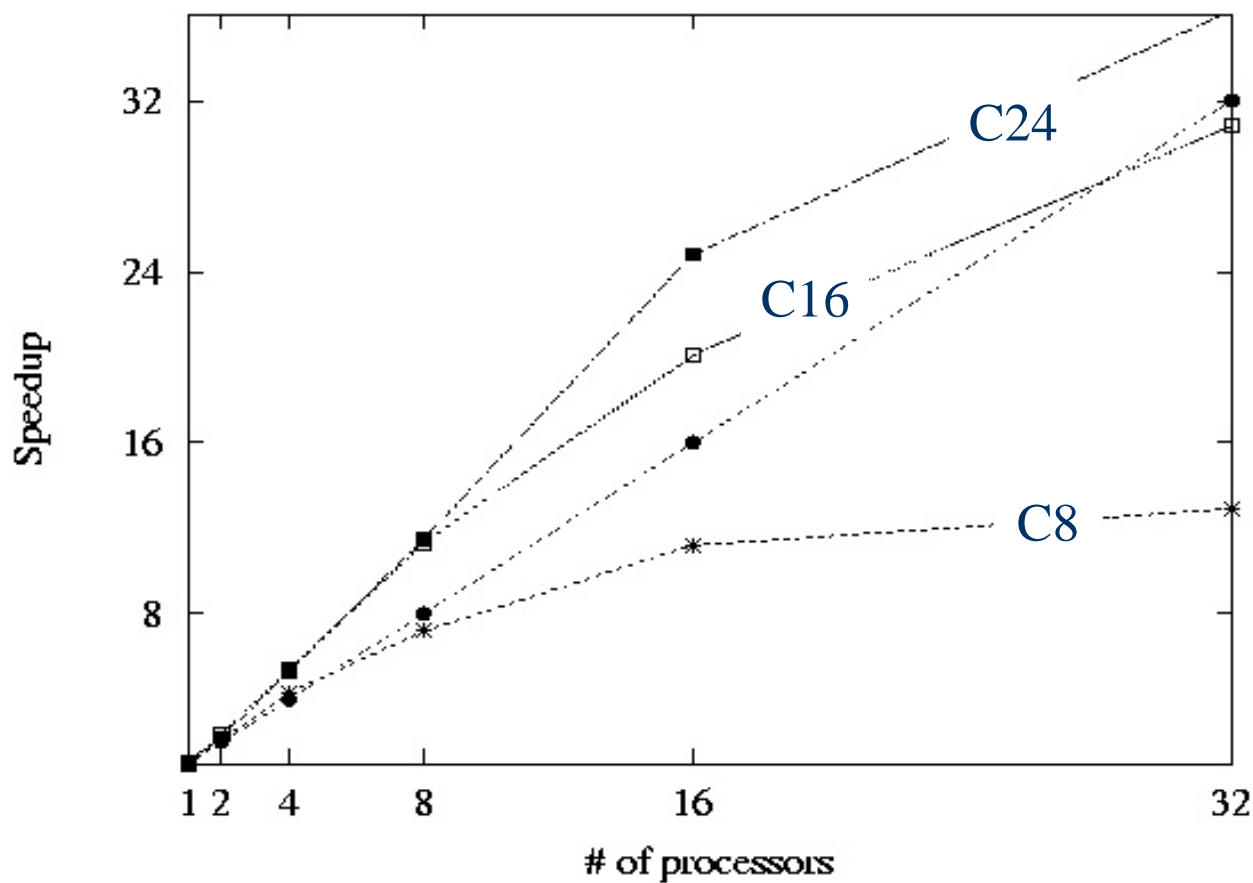
- Up to 2nd derivatives for HF and DFT
- Including linear scaling J-engine, CFMM and FTC
- Distributed memory for frequency calc
- Available on all the platforms
- Mol. Phys. **100**, 1755 (2002)

Parallel Speed-up on IBM SP DFT Energy and Gradient



Job: Taxol, 6-31G*, BLYP, 1032 basis functions.

CPHF speedup for alkane series in Q-CHEM on PC Linux cluster



Developer: *Shawn Brown*

“incdft = 1”

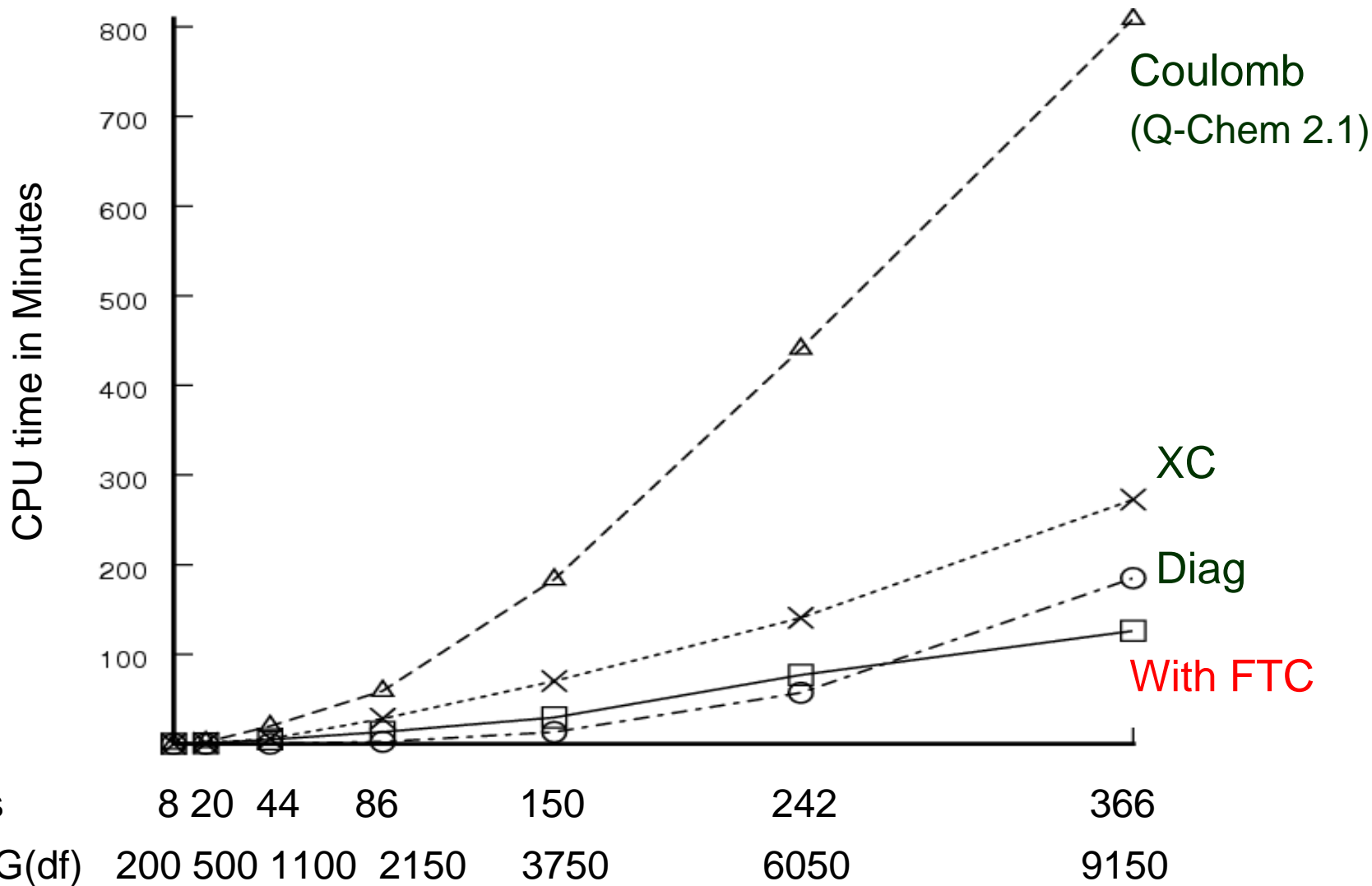
- Takes the advantage of small differences between SCF cycles
- Can be combined with variational threshold
- Double the speed for the numerical integration of XC
- CPL, **408**, 395 (2005)

Developer: *Laszlo Fusti-Molnar*

“ftc = 1”

- Calculates the integrals with diffuse functions
- $O(N^2)$ in basis set size versus $O(N^4)$
- $O(N)$ in system size with a small crossover
- No loss of accuracy
- Fusti-Molnar, Kong, *JCP*, **122**, (2005).

Fourier Transform Coulomb

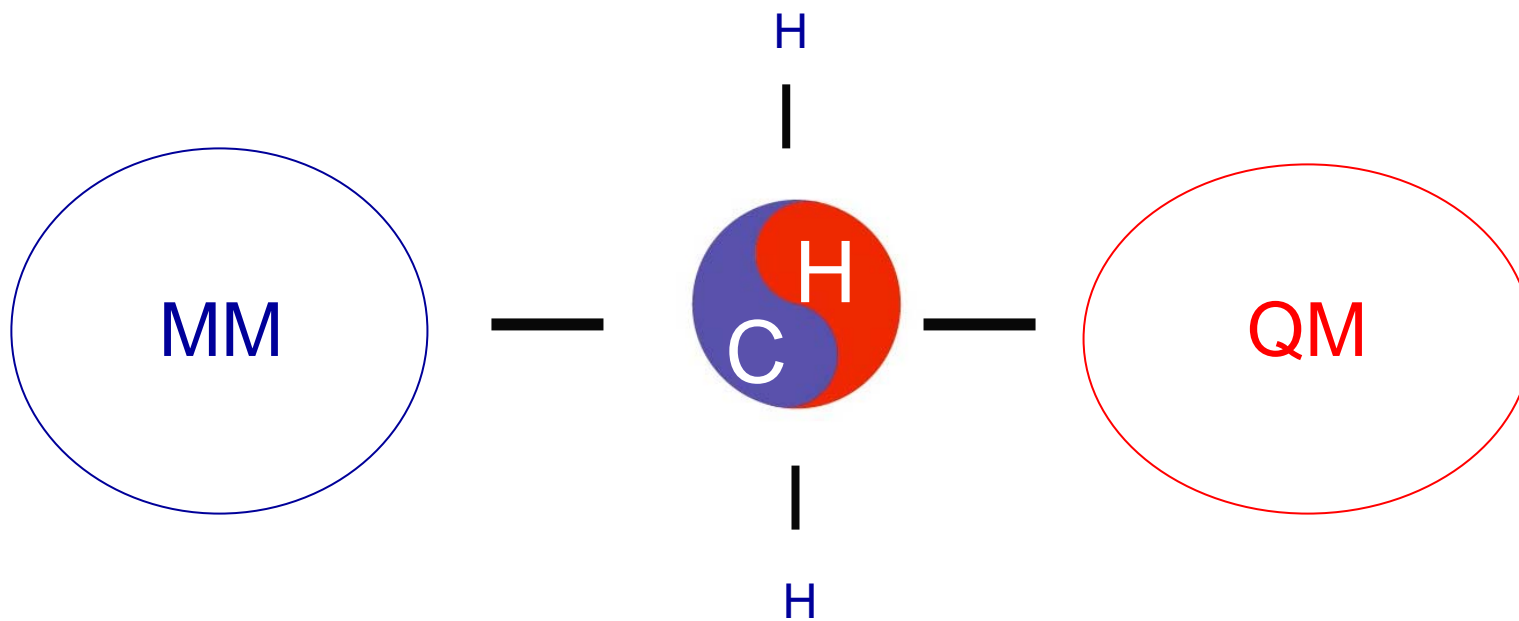


Developer: *Yihan Shao*

“qmmm_interface yinyang”

“force_field charmm27”

- Extremely simple: ONE parameter!
- Trivial to implement
- As accurate as any other model

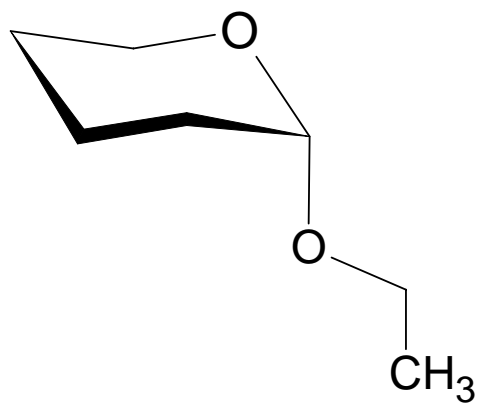
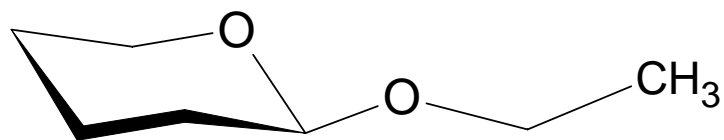


Developers: Gan, Proynov

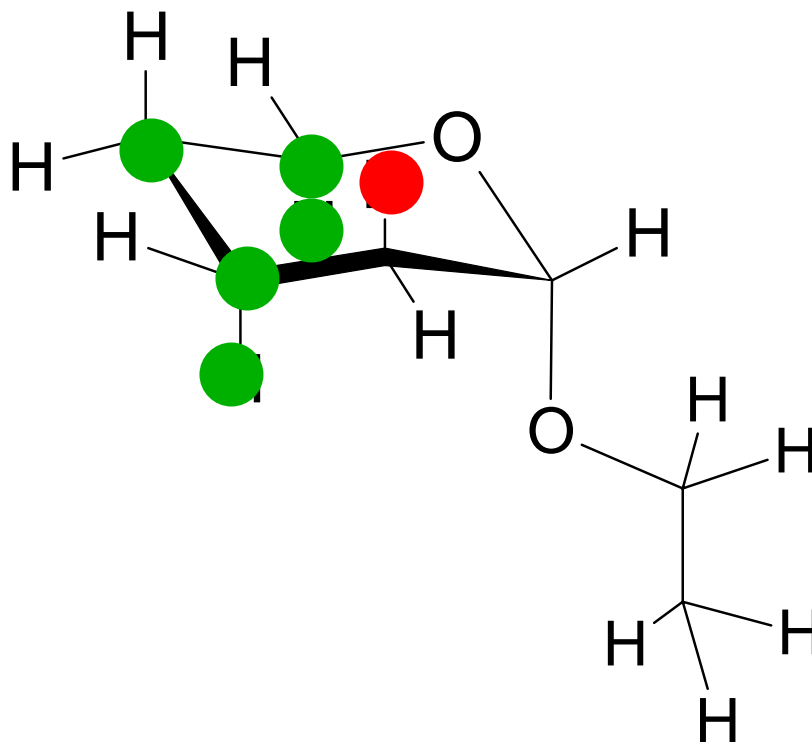
To be released:

- Based on Becke&Johnson's exchange-hole dipole moment (XDM) model
- Calculates dispersion electronically
- Our implementation:
 - SCF and analytical gradients
 - Efficient: Little extra cost
 - Phys. Rev. A, submitted

Pyran as the model for the glycosidic linkage



ccpVTZ Basis	$E_{\text{eq}} - E_{\text{ax}}$ (kcal/mol)
Experiment	(0.47 ± 0.3)
CCSD(T)	1.47 (0.49)
B3LYP	0.63 (-0.12)
B3LYP+XDM	1.07 (0.32)



www.q-chem.com

Current:

Yihan Shao
Emil Proynov
Zhengting Gan
Nick Russ
Chunmin Chang
ZitaAnn Berry
Hilary Pople
Jaime Martell

Past:

Shawn T. Brown @ PSC
Holger Dachsel @ Julish
Fusti-Molnar @ Florida
Prakashan Korambath @ UCLA
Weimin Zhang @ ScottTrade

Collaborators:

Tom Furlani and Marek Freindorf
at Univ. Buffalo

