

quadrature grid improvements

"same accuracy. faster computation"

grid pruning

Isotropic density close to the nuclei. Less dense grid needed.

- atomic spherical grid divided into regions. Different Lebedev order for each region.

New PSI4 options:

```
set DFT_PRUNING_SCHEME ROBUST
```

```
set DFT_PRUNING_SCHEME TREUTLER
```

grid pruning

- ROBUST = sphere divided into quarters

	Lebedev order (spherical part)	1st (innermost)	2nd	3rd/4th	total points for Carbon	reduction
scheme	[n]	[7]	[n-6]	[n]		
"UltraFine" 590/99 grid	41	26 [7]	434 [35]	590 [41]	36844 -> 54280	32 %

grid weights screening

grid points with small quadrature weights can be neglected

New PSI4 option:

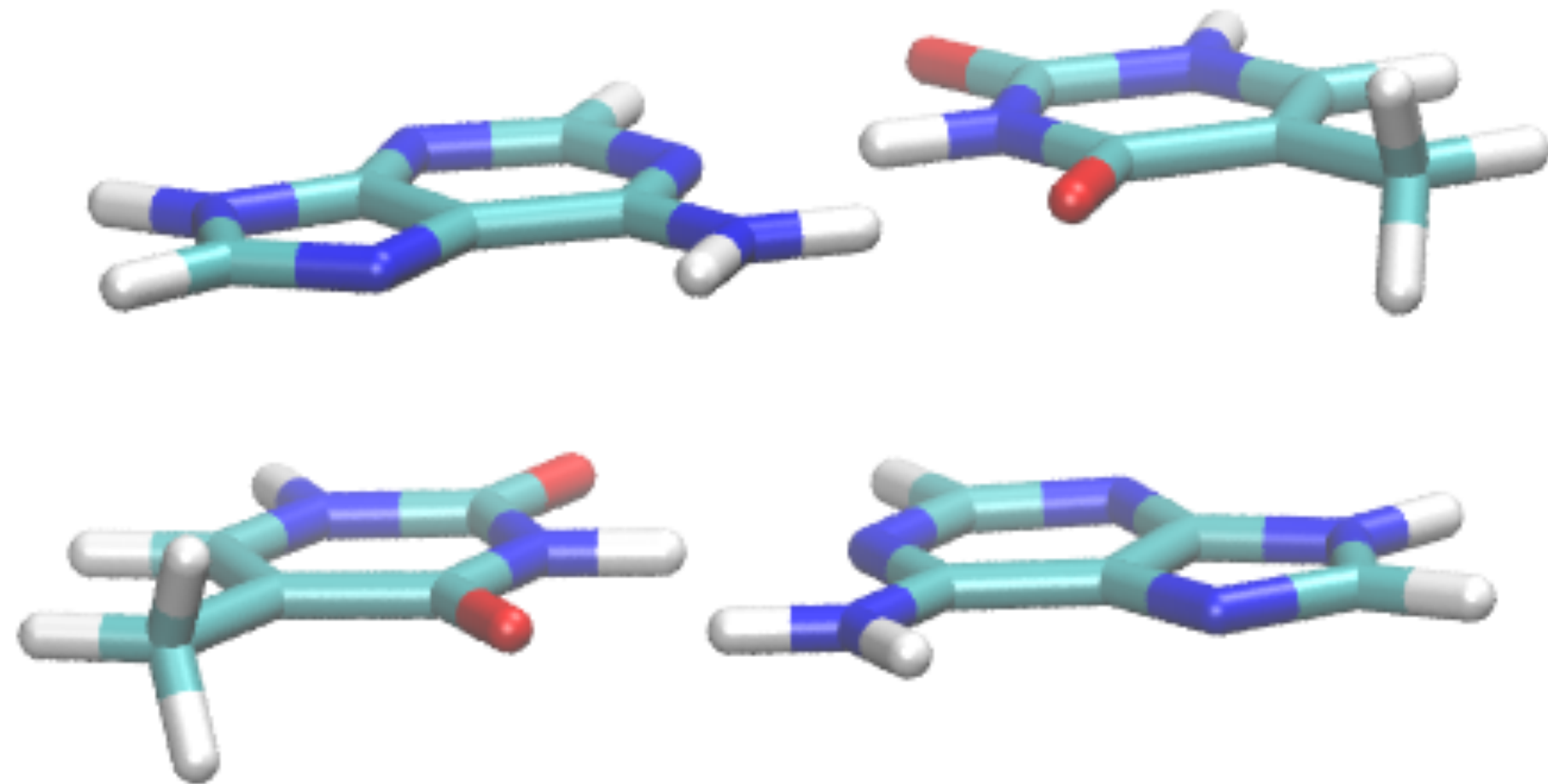
```
set DFT_WEIGHT_TOLERANCE 1e-15
```

new grid defaults

grid weight screening: `set DFT_WEIGHT_TOLERANCE 1e-15`

grid pruning: `set DFT_PRUNING_SCHEME ROBUST`

ApT base-pair step



PBE0-D3BJ/def2-TZVP; 590/99 UltraFine grid; 16 threads

	no pruning	pruning
total points	3489564	2085560
timing	4.7 min	3.2 min