

H2 molecule :



Delley partition-tab

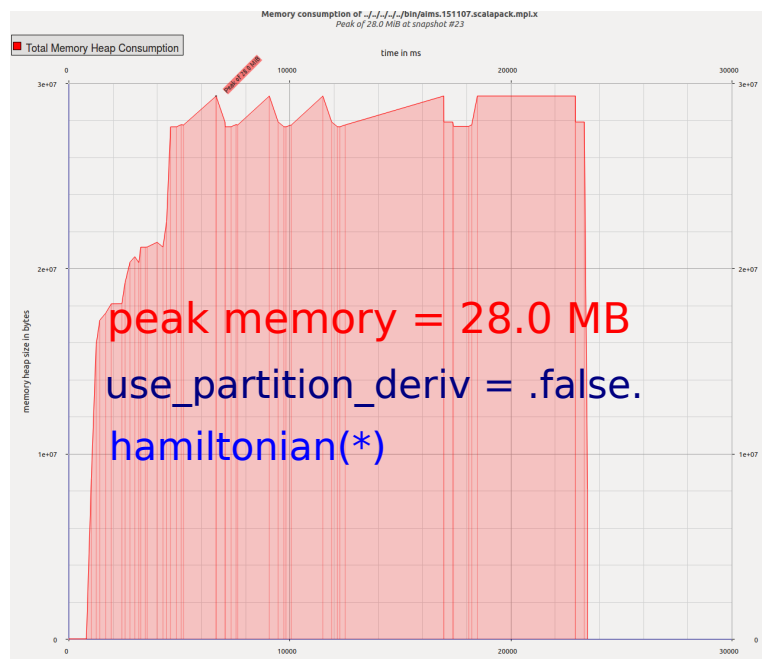
Basis set: minimal

Grid: tight setting

XC : LDA

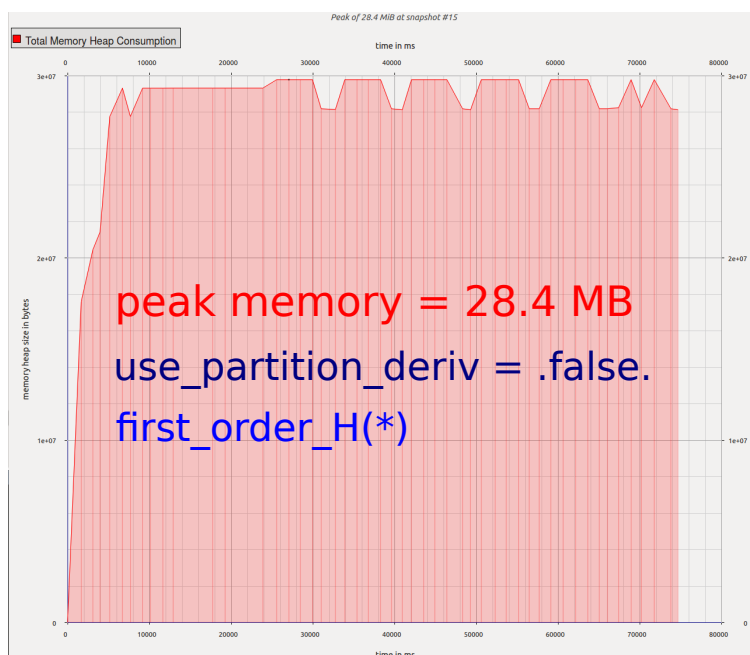
(1) DFT

(Time = 22 000 ms)



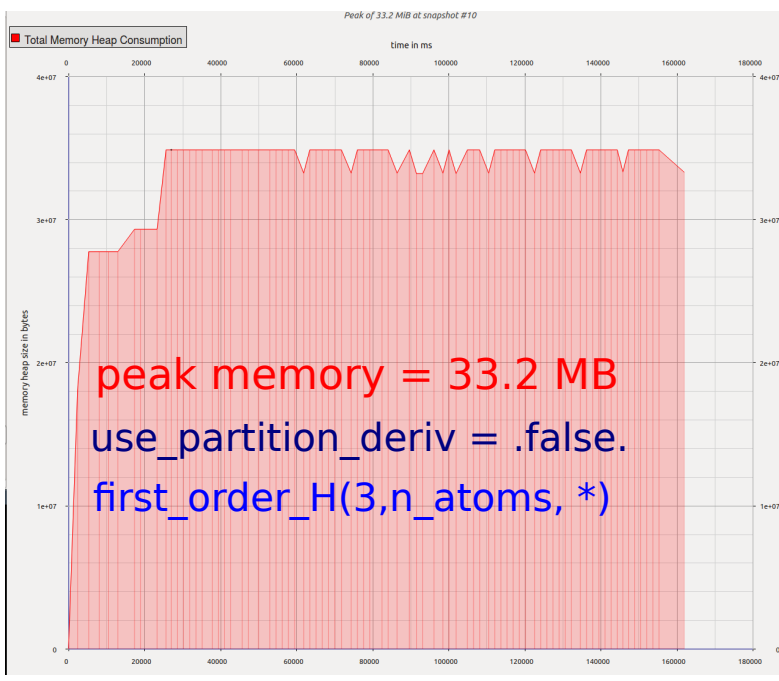
(2) DFPT vibration_reduce_memory

(Time = 73 000 ms)



(3) DFPT vibration

(Time = 161 000 ms)



(4) DFPT vibration_with_moving_grid_effect

(Time = 169 000 ms)

