

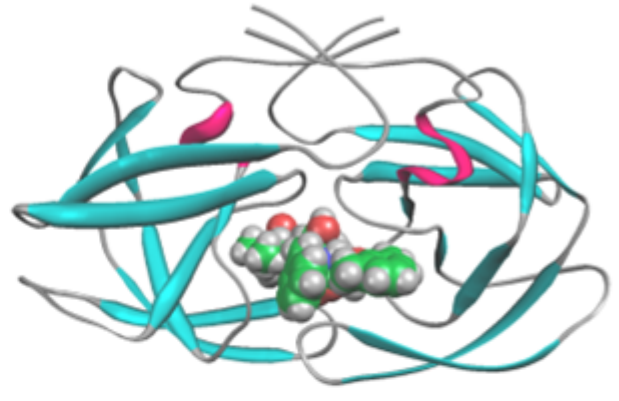
FMOプログラムABINIT-MPの高速化と超大規模系への対応

課題代表者: 望月祐志(立教大) / 共同研究者: 中野達也(国立衛研)、坂倉耕太(FOCUS)、渡邊啓正(HPCS)、片桐孝洋、大島聡史、満田晴紀(名大)、森脇吉隆(東大)、杉崎研司(阪公大)

FMO Original Ref.: K. Kitaura et al., Chem. Phys. Lett. 313 (1999) 701 / General Ref.: M. Gordon et al., Chem. Rev. 112 (2012) 632.

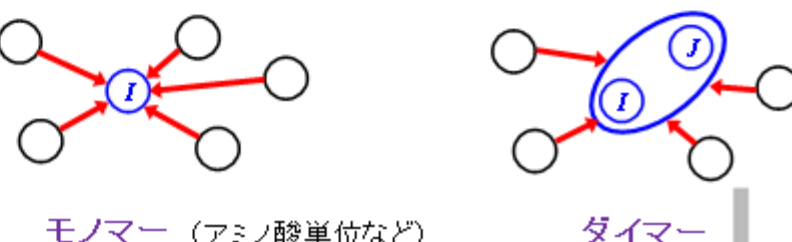
フラグメント分子軌道(FMO)法

◇巨大分子系
生体高分子や凝集系では一般的
⇒ タンパク質、DNA (水和状態)
数千~数万原子、数千~数十万軌道

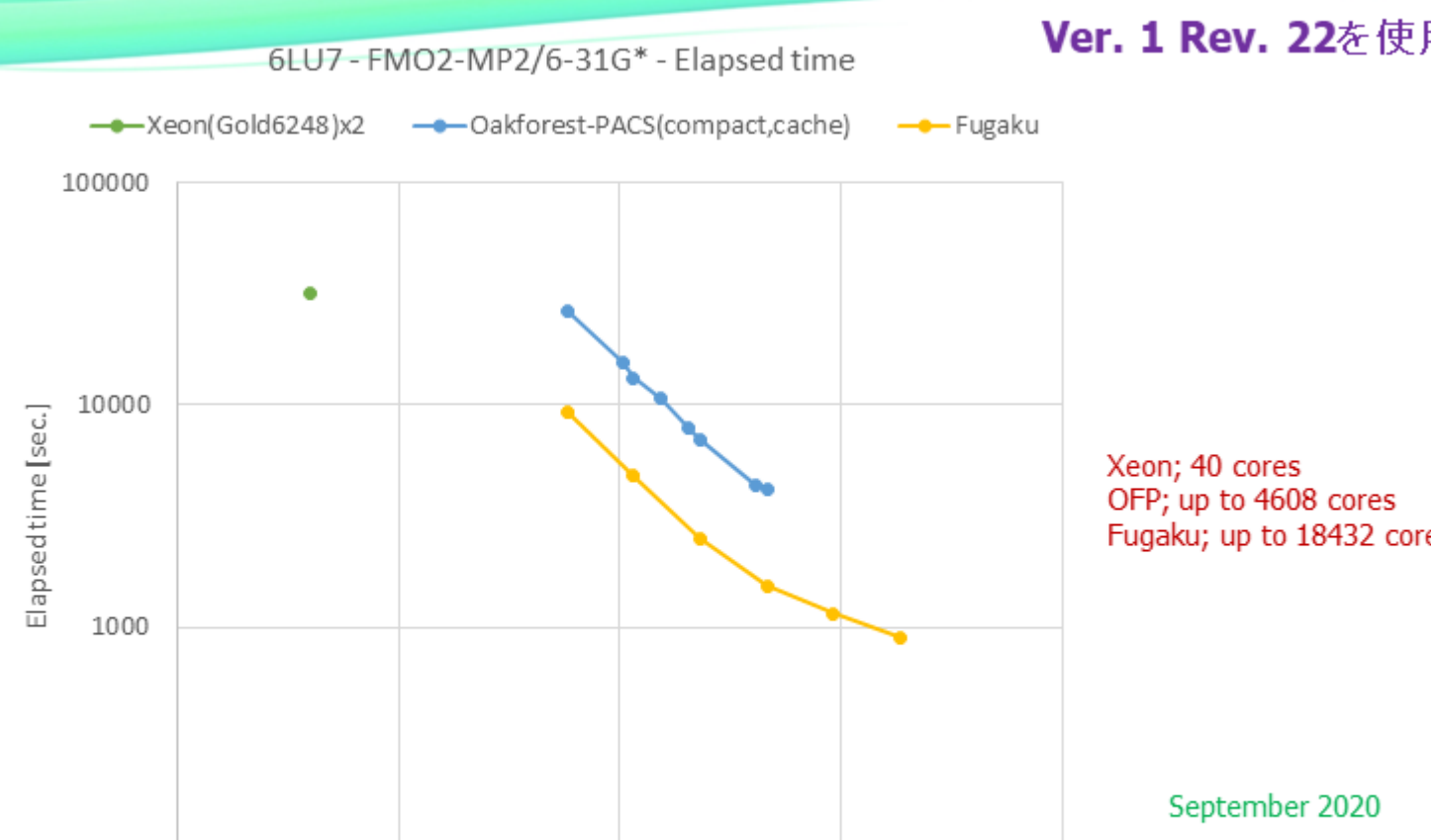


◇分割&統合系のアプローチの一つ
北浦らが23年程前に2体展開で提案

- ⇒ フラグメントとその対系のエネルギーを評価 (FMO2)
 - ⇒ 環境静電ポテンシャル (ESP)、直接結合切断 (BDA)
 - ⇒ 階層的な並列処理 (フラグメントリスト&内部処理)
 - ⇒ 定量性を高める電子相関の導入も直截
- フラグメント間の相互作用エネルギー (IFIE)
- ⇒ 計算対象の解析ツール
 - ⇒ 生物物理や創薬に向く
 - ⇒ 材料系にも適用可能



FMO-MP2/6-31G*ジョブのスケールアップ



- PDB ID: 6LU7 = SARS-CoV-2 Mpro + N3 ligand の系
- MP2の積分変換は全てDGEMMで実行
- Dimer-ESのCMM近似は (>5のリージョンで使用)
- 「富岳」はOakforest-PACSよりも2.8倍ほど速い

A64FX向けの高速化

- 2電子積分の生成
 - {SSSS, PSSS, SPSS, SSPS, SSSP, PPSS, PPS, PPS, SPPS, SPS, SSSP, DSSS, SDSS, SSDS, SSSD}の積分タイプを(手動で)SIMD化
 - OCL指示詞の追加
 - コンパイラオプション: -O3 -Knosmid -Kocl
 - 改良の効果は20~30%程度 (幾つかの系でテスト: jh210036-NAH課題で実施)
 - 最新リリースのVer. 2 Rev. 4に反映 (「GUIのみ配列」の削除も: 大規模系対応)

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