Task-Based Parallel Computation of the Density Matrix in Quantum-Based Molecular Dynamics using Graph-Partitioning

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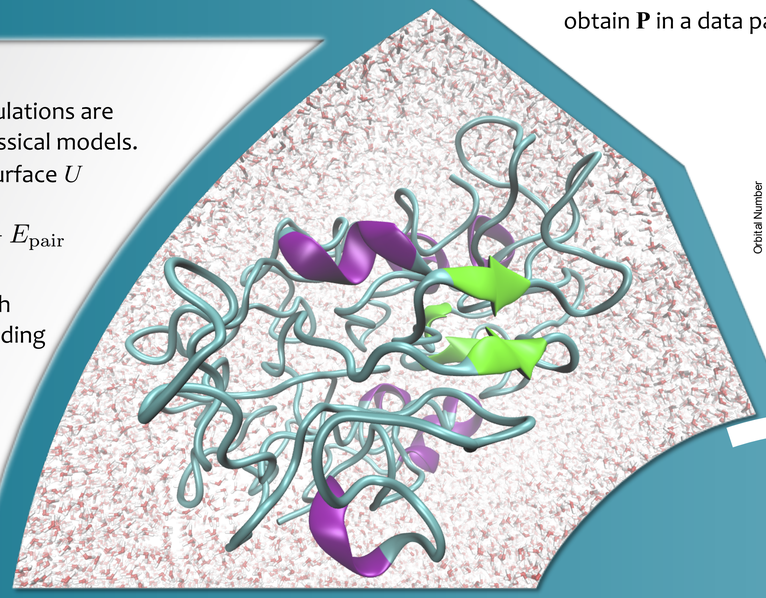
Motivation

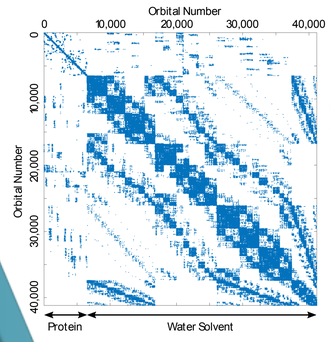
Quantum-based molecular dynamics (QMD) simulations are substantially more accurate than those using classical models. QMD trajectories evolve on a potential energy surface U

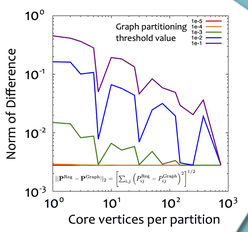
$$U = 2\mathrm{Tr}\left[\left(\mathbf{P}-\mathbf{P}^0\right)\mathbf{H}\right] - \tfrac{1}{2}\sum_{i,j=1}^{N}\gamma_{ij}q_iq_j + E_{\mathrm{pair}}$$

that depends on the Hamiltonian matrix $\mathbf{H}$, which represents chemical bonding, and the corresponding electron density matrix $\mathbf{P}$.[1] Obtaining $\mathbf{P}$ from $\mathbf{H}$ is the most expensive computational step. Traditional O(N^3) matrix diagonalization limits the number of simulated atoms N to ~1000. Our goal is to use QMD for large systems (N > 10,000), such as solvated proteins.



QMD simulations depend on quickly computing $\mathbf{P}$ from $\mathbf{H}$. We investigate graph partitioning to obtain $\mathbf{P}$ in a data parallel implementation of SP2.





Second-Order Spectral Projection (SP2)

SP2 is an efficient, O(N) method to obtain $\mathbf{P}$ for non-metallic systems, replacing O(N^3) diagonalization with a polynomial expansion of $\mathbf{H}$.[2] SP2 scales best when $\mathbf{H}$ and $\mathbf{P}$ are sparse.

$$\mathbf{P} = \theta\left[\mu\mathbf{I}-\mathbf{H}\right] = \lim_{i\to\infty} f_i\left[f_{i-1}\left[\ldots f_0\left[\mathbf{X}_0\right]\ldots\right]\right]$$

$$f_i\left[\mathbf{X}_i\right] = \begin{cases} \mathbf{X}_i^2 & \text{if } 2\mathrm{Tr}\left[\mathbf{X}_i\right] \geq N_{\mathrm{e}} \\ 2\mathbf{X}_i - \mathbf{X}_i^2 & \text{if } 2\mathrm{Tr}\left[\mathbf{X}_i\right] < N_{\mathrm{e}} \end{cases}$$

$$\mathbf{X}_0 = \frac{\epsilon_{\max}\mathbf{I}-\mathbf{H}}{\epsilon_{\max}-\epsilon_{\min}}$$

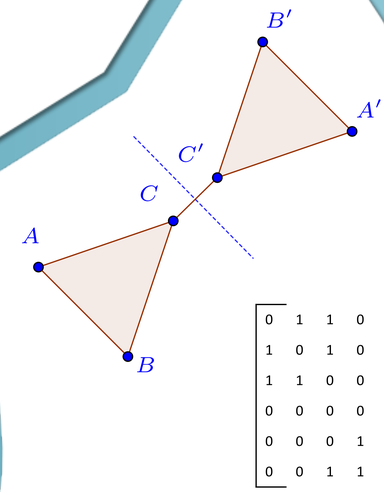
Graph Partitioning

Traditional graph partitioning approaches minimize edge-cut between partitions.

To account for inter-partition interactions, we extend existing approaches to reduce the size of partitions with respect to both the number of vertices per partition as well as the number of neighbor vertices in adjacent partitions.

Denoting the number of nodes per partition as c and the number of neighbor vertices as h, we reduce the matrix operation costs for the SP2 method summed over all the partitions P:

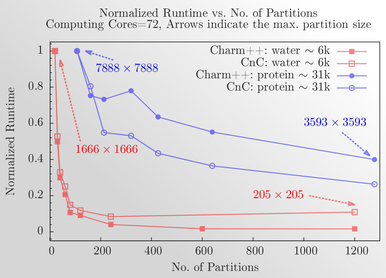
$$\sum_{i\in P}(c_i+h_i)^3$$

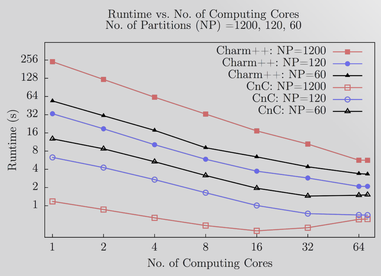


$$\begin{bmatrix} 0&1&1&0&0&0\\ 1&0&1&0&0&0\\ 1&1&0&0&0&1\\ 0&0&0&0&1&1\\ 0&0&0&1&0&1\\ 0&0&1&1&1&0 \end{bmatrix}$$

We first represent $\mathbf{P}$ from the last QMD time step as an undirected graph: basis orbitals (such as *s* and *p*) are vertices and non-zero elements are edges.

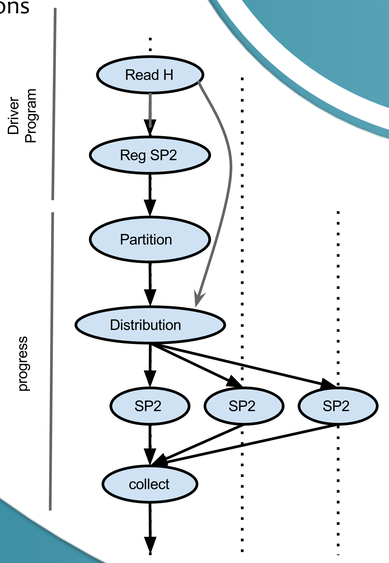
Task-Based Parallel Implementation

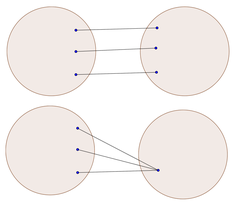




Undesirable load-imbalances can arise as the partitions are not of equal size. Asynchronous task-based programming models, such as CnC and Charm++, mitigate load-balancing problems typical of MPI/OpenMP implementations by efficiently scheduling computations at runtime.

Intel Concurrent Collections[4] (CnC) and Charm++[5] implementations exploit the independent sub-problems resulting from our graph partitioned approach to SP2 and are integrated into an existing QMD code.





Protein: 31941 orbitals, 64 partitions.

method	$\sum_{i\in P}(c_i+h_i)^3$
blocking	1791576117859
hMETIS	346007029558
hMETIS+SA	311427370057

A naive approach to divide $\mathbf{H}$ into sub-problems (blocking) is not efficient. Applying classical graph partitioning tools (*hMETIS*)[3] to $\mathbf{P}$ performs better, but is not optimal for our purpose. Post-processing with simulated annealing (SA) can refine this result.

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The poster design was adapted from the designs of Felix Breuer.
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