A quantum chemistry calculation distributed among computing facilities with Quantum Package

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October 2019

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\textsuperscript{2}CRIANN: Centre Régional Informatique et d’Applications Numériques de Normandie, Saint-Étienne-du-Rouvray
\textsuperscript{3}CALMIP: Calculs en Midi-Pyrénées, Toulouse
Abstract
We have shown we are able to make \textit{routinely} distributed calculations for quantum chemistry using 20 nodes of CRIANN and 20 nodes CALMIP.

Outline

- Presentation of the method
  - Selection
  - Davidson’s iterations
- Parallelism / Experimental setup
- Results
  - Selection
  - Davidson’s iterations
Scientific problem: Schrödinger’s equation

\[ H \Psi = E \Psi \quad ; \quad \Psi = \sum_{i=1}^{N_{\text{det}}} \Psi_i D_i \]

Find the best possible approximation of \( \Psi \) and \( E \)

- Find approximate lowest eigenpair(s) and of the Hamiltonian matrix \( H \)
- \( N \) can be as large as \( 10^{30} \) for small molecules (exponential scaling)
- Eigenvector(s) and eigenvalue(s) of an approximate Hamiltonian \( \tilde{H} \)
- \( N \) must be reduced to less than \( \sim 10^9 \) by choosing appropriate Slater determinants \( D_i \)
CIPSI Algorithm

\[ \mathbf{H} \mathbf{\Psi} = E \mathbf{\Psi} \; ; \; \mathbf{\Psi} = \sum_{i=1}^{N_{\text{det}}} \mathbf{\Psi}_i \mathbf{D}_i \]

1. Start with \( n = 0, \mathbf{\Psi}^{(n)} = \mathbf{D}_0 \)
2. **Selection**: Identify a new set \( \mathcal{D}_n = \{ \mathbf{D}_i \} \) which are likely to have a large contribution \( \mathbf{\Psi}_i \)
3. Extend the vector space \( (\bigcup_{m<n} \mathcal{D}_m) \cup \mathcal{D}_n \):
4. **Davidson’s algorithm**: Find the pair \( \mathbf{\Psi}^{(n+1)}, E^{(n+1)} \), the lowest root of \( \mathbf{H} \) in the new vector space
5. Go to 2.
MPMD: Multiple Program / multiple data

- One executable: the task scheduler
- One executable: the master compute process (OpenMP)
- One/Many executable(s): slave compute processes (MPI/OpenMP, 1 process/node)
- One process to tunnel data through different networks
- Inter-process communication with ZeroMQ
Task-based Parallelism

Design

Master

Slave

Tunnel

Motivations

• Possibility to increase dynamically computational resources
• Fault tolerance
• Possibility to use cloud infrastructures
Each task is computed with all possible OpenMP threads.
Experimental setup
Results: Measurements

Bandwidth
- CALMIP login ↔ CALMIP compute: IB EDR 100Gb/s
- CRIANN login ↔ CALMIP login: Renater: 74.1 MB/s
- CRIANN login ↔ CRIANN compute: Omnipath 100GiB/s

Latency (ping)
- CALMIP login ↔ CALMIP compute: 0.09 ms
- CRIANN login ↔ CALMIP login: 16.72 ms
- CRIANN login ↔ CRIANN compute: 0.23 ms
Results: Davidson’s diagonalization

- Size of the vectors: \( N = 21\,691\,814 \), 109 tasks
- 412 MiB sent to each MPI group at the beginning
- 165 MiB sent to each MPI group per Davidson iteration
- 1.5 MiB as a result of a task
- Starting from a bad guess: \([1 \ 0 \ldots \ 0 \ 0]\) → 17 iterations

<table>
<thead>
<tr>
<th>Configuration</th>
<th>( N_{\text{CPU}} )</th>
<th>Wall time</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 nodes Olympe</td>
<td>1440</td>
<td>36:51</td>
</tr>
<tr>
<td>40 nodes Myria</td>
<td>1120</td>
<td>44:10</td>
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<td>20 nodes Myria, 20 nodes Olympe</td>
<td>1280</td>
<td>43:48</td>
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</tbody>
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Results: Selection

- Size of the vectors: $N = 21 \, 691 \, 814$, $21 \, 854 \, 665$ tasks
- Stop when relative error is 0.1% $\rightarrow \sim 3\%$ of the tasks
- 412 MiB sent to each MPI group at the beginning
- Each task returns 40 bytes
- Each ZeroMQ client fetches $m$ tasks, where $m$ is dynamically adjusted such that the computation of the $m$ tasks takes $\sim N_{CPU}$ seconds.
- The next $m$ tasks are prefetched during the current computation

<table>
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<tr>
<th>Configuration</th>
<th>$N_{CPU}$</th>
<th>Wall time</th>
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<tbody>
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<td>25 nodes Myria, 25 nodes Olympe</td>
<td>1600</td>
<td>13:19</td>
</tr>
</tbody>
</table>
Improving Results

Sould we re-try the experiment now?
Quantum Package

https://quantumpackage.github.io/qp2
https://github.com/QuantumPackage/qp2

- Open-source program\textsuperscript{1} developed at LCPQ and LCT (Paris)
- Wave function methods for extreme accuracy (benchmarks)
- Computational goal: make wave function methods scalable

https://arxiv.org/abs/1902.08154