Offloading to GPUs with OpenMP: Case Study with GAMESS

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  - Peng Xu
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  - JaeHyuk Kwack

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INTRO OF GAMESS

- GAMESS is the General Atomic and Molecular Electronic Structure System
  - General-purpose electronic structure code (many methods and capabilities)
  - ~1 million lines of Fortran
  - Optional C/C++ GPU-accelerated libraries/applications in GAMESS

- Scientific problem of interest
  - FMO/RI-MP2 calculations towards accurate simulations of catalysis reactions inside a mesoporous silica nanoparticle
GAMESS ON GPUS

- Several methods ported to GPUs
  - Hartree-Fock
    - Solves a set of non-linear eigenvalue equations iteratively
    - Two main bottlenecks: 1) computation of a very large number of 4-index 2-electron repulsion integrals (4-2ERIs); and 2) forming a $N^2$ Fock matrix by contracting the $N^4$ 4-2ERI tensor with a density matrix.
  - RI-MP2
    - Correction to Hartree-Fock
    - RI approximation simplifies the integral evaluation from 4-index to 3-index 2-electron repulsion integrals and allows the use of efficient matrix multiplication operations
GPU BACKGROUND
VERY BRIEF GPU HARDWARE INTRO

Nvidia V100 (GPU on Summit)

- V100s have hierarchical parallelism (SMs and CUDA cores in an SM)
- Threads execute lock-step in a warp
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HARTREE-FOCK PORTING
INTRO OF HF: CPU VERSION

- Focused on the 4-2ERI evaluation since they are a main computational bottleneck
- Parallelized previously with MPI+OpenMP CPU threading
  - But multiple levels of conditional statements and load imbalance between threads

```fortran
subroutine compute_integrals ( ... )
    ! bottleneck loop over N^4 4-2ERIs
    !$omp parallel do private ( ... )
    do i=1, N^4
        ! branching over methods
        if (method(i) .eq. 1 ) call method_one(i)
        if (method(i) .eq. 2 ) call method_two(i)
        ...
    enddo
    ...
end subroutine compute_integrals

! routine for specific integral method
subroutine method_one( i )
    ...
    ! branch again on integral type
    if ( type(i) .eq. 1 )
        call int1 ( i, ...)
    ...
end subroutine method_one
```
INTRO OF HF: CPU VERSION

```fortran
subroutine compute_integrals(...) ! bottleneck loop over \( N^4 \) 4-2ERIs
   !$omp parallel do private(...) do i=1, \( N^4 \)
     ! branching over methods
     if(method(i) .eq. 1) call method_one(i)
     if(method(i) .eq. 2) call method_two(i)
     ...
   enddo
   ...
end subroutine compute_integrals

! routine for specific integral method
subroutine method_one(i)
   ...
   ! branch again on integral type
   if(type(i) .eq. 1) call int1(i, ...)
   ...
end subroutine method_one
```

```fortran
subroutine compute_integrals(...) do i=1,\( N^4 \)
   ! create sorted array by method and type
   if(method(i) .eq. 1 .and. type(i) .eq. 1) store i in sorted(method=1,type=1)
   endif
   ...
enddo
!
! after sorting, integrals of different methods and
! types are evaluated separately
!$ omp target teams distribute parallel do map(...)
do i in sorted(method=1,type=1)
   call int1(i, ...)
enddo
!
!$ omp target teams distribute parallel do map(...)
do i in sorted(method=1,type=2)
   call int2(i, ...)
enddo
...
end subroutine compute_integrals
```
### RESULTS AND ISSUES

- Cluster of N water molecules.
- Using 6-31G basis set [SP only for now]

<table>
<thead>
<tr>
<th>N</th>
<th>Wall time CPU (s)</th>
<th>Wall time GPU (s)</th>
<th>Speedup</th>
<th>#QUARTETS</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>0.1</td>
<td>3.0</td>
<td>&lt;0.1</td>
<td>51,519</td>
</tr>
<tr>
<td>8</td>
<td>0.1</td>
<td>5.3</td>
<td>&lt;0.1</td>
<td>548,454</td>
</tr>
<tr>
<td>16</td>
<td>1.0</td>
<td>7.7</td>
<td>0.1</td>
<td>3,899,510</td>
</tr>
<tr>
<td>32</td>
<td>18.0</td>
<td>16.3</td>
<td>1.1</td>
<td>24,078,056</td>
</tr>
<tr>
<td>48</td>
<td>102.0</td>
<td>18.0</td>
<td>5.7</td>
<td>65,325,492</td>
</tr>
<tr>
<td>64</td>
<td>243.0</td>
<td>26.0</td>
<td>9.3</td>
<td>128,650,354</td>
</tr>
</tbody>
</table>

- For GPU calculations: 1 MPI rank, 42 threads, 1 GPU.
- For CPU calculations: 1 MPI rank, 42 threads.
- N is the number of water molecules in water cluster.
- W.t. CPU is the recorded wall time (s) of quartet formation and Fock build for 1 SCF iteration using CPU threaded code.
- W.t. GPU is the recorded wall time (s) of quartet formation and Fock build for 1 SCF iteration using GPU+CPU threaded code.
- Speedup is the ratio of w.t. CPU over w.t. GPU.
RESULTS AND ISSUES

Issues

1. We found that if we had a function call in an offloaded target region and were also using thread-local arrays, our runtime increased with increasing iterations.

2. We found that using thread local arrays hurt performance. When we made thread-local arrays ourselves (and indexing by thread ourselves), the issue went away.

Reported to Oak Ridge/IBM support
RI-MP2 PORTING
INTRO OF RI-MP2 MINI-APP

- Computes RI-MP2 perturbative correction to the Hartree-Fock energy

- RI approximation allows the integral evaluation to be simplified and written in terms of matrix multiplication

\[
E^{(2)} = \sum_{i \leq j} (2 - \delta_{ij}) \sum_{ab} \frac{(ia|jb)[2(ja|jb) - (ib|ja)]}{\epsilon_i + \epsilon_j - (\epsilon_a + \epsilon_b)}
\]

\[
(ia|jb) = \sum_P B_{ia}^P B_{jb}^P
\]
INTRO OF RI-MP2: CPU VERSION

- Focused on the computation of the perturbative correction, since it is the main bottleneck of the RI-MP2 method

- Majority of the time is spent in a DGEMM (matrix multiply) call

```plaintext
int do JACT=1, NACT
  do IACT=1, JACT
    ... 
    call RIMP2_EIJ( B32(:,; , IACT), B32(:,; , JACT), ...)
  enddo
endo
d odo
  subroutine RIMP2_EIJ( ... )
... 
  call DGEMM with BI(:,;), BJ(:,;), QVV(:,;)
do IB=1,NVIR
  do IA=1,NVIR
    compute E2_{t} with QVV(:,;), ... 
  enddo
endo
... 
end subroutine
```
do JACT=1, NACT
  do IACT=1, JACT
    ...  
call RIMP2_EIJ( B32(:,:, IACT), B32(:,:, JACT),...)
  enddo 
enddo
subroutine RIMP2_EIJ( ... )
...  
call DGEMM with BI(:,:,), BJ(:,:,), QVV(:,:,)
do IB=1,NVIR
  do IA=1,NVIR
    compute E2.t with QVV(:,:,), ...
  enddo
enddo
...
end subroutine
RESULTS AND ISSUES

Table 10. Walltimes and Speedups of the restructured RI-MP2 kernel (input: c60.kern)

<table>
<thead>
<tr>
<th>Directives</th>
<th>Math Library</th>
<th>Processors</th>
<th>Wall time (sec)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serial</td>
<td>ESSL</td>
<td>1 core of an IBM Power9</td>
<td>342.697</td>
<td>0.036 x</td>
</tr>
<tr>
<td>OpenMP threading</td>
<td>ESSL</td>
<td>2 IBM Power9 (42 threads)</td>
<td>12.231</td>
<td>1 x</td>
</tr>
<tr>
<td>OpenMP threading</td>
<td>MKL</td>
<td>2 Intel Xeon 8180M (112 threads)</td>
<td>4.317</td>
<td>2.83 x</td>
</tr>
<tr>
<td>OpenMP Offloading</td>
<td>NVBLAS</td>
<td>1 NVIDIA V100</td>
<td>1.734</td>
<td>7.05 x</td>
</tr>
<tr>
<td>OpenMP Offloading</td>
<td>cuBLAS</td>
<td>1 NVIDIA V100</td>
<td>1.983</td>
<td>6.17 x</td>
</tr>
<tr>
<td>OpenMP Offloading</td>
<td>cuBLASXT</td>
<td>1 NVIDIA V100</td>
<td>1.728</td>
<td>7.08 x</td>
</tr>
<tr>
<td>OpenACC Offloading</td>
<td>cuBLAS</td>
<td>1 NVIDIA V100</td>
<td>1.905</td>
<td>6.42 x</td>
</tr>
<tr>
<td>OpenACC Offloading</td>
<td>cuBLASXT</td>
<td>1 NVIDIA V100</td>
<td>1.692</td>
<td>7.23 x</td>
</tr>
</tbody>
</table>

J. Kwack, C. Bertoni, B. Pham, J. Larkin, WACCPD ‘19
RESULTS AND ISSUES

Issues

- Vendor library interoperability with OpenMP
TAKE-AWAYS

- Think about GPU architecture and how to write efficient code on it

- OpenMP (IBM 16.1) had all of the features we wanted
  - Some issues: unexpected slow performance for some features and interactions with vendor math libraries
  - But overall, with OpenMP we achieved reasonable speedups over the CPU versions

- Coming in OpenMP 5.1
  - Dispatch construct!
For the OpenMP specification, tutorials, forum, reference guides, and links to other resources, visit www.openmp.org