Optimizing Two-Electron Repulsion Integral Calculation on Knights Landing Architecture

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Outline

- Background & Mathematics
- Algorithm
- Benchmark Result

Background: Quantum Chemistry

- Quantum chemistry programs are the most used programs on our supercomputer.
- One hotspot for quantum chemistry software is the two-Electron Repulsion Integral (ERI).

Rank	Program
1	VASP
2	GAUSSIAN
3	Material Studio
4	MOLPRO
5	NWChem

Top 5 most used programs on CAS supercomputer.
Consumes 20% of total CPU hours.

ERI Mathematical Formula

- The mathematical formula of primitive ERI is:

$$[is|jt] = \iint_{-\infty}^{\infty} \varphi_{\mathrm{i}}^{*}(r_1)\varphi_s^{*}(r_2)\frac{1}{r_1 - r_2}\varphi_j(r_1)\varphi_t(r_2)dr_1dr_2$$

  - $\varphi_{\mathrm{i}}^{*}(r_1)$ is the complex conjugate of $\varphi_i(r_1)$. Here all functions are real, so $\varphi_{\mathrm{i}}^{*}(r_1) = \varphi_i(r_1)$.

- $\varphi_i(r_1)$ is gaussian type function with different angular momentum L:

$$\varphi_i(r_1) = (x_1 - x_i)^n(y_1 - y_i)^l(z_1 - z_i)^m \exp(-\alpha_i(r_1 - r_i)^2), \qquad n + l + m = L$$

- The main purpose of ERI is to calculate all the primitive integrals for a given set of $\varphi(r)$ functions.
- So if you have N number of functions, the total number of ERI calculation is N^4. Normally N is around 100s~1000s.
- Integral calculations are independent.

Gaussian Product Theorem

- The Gaussian product theorem is :

$$\exp(-\alpha_i(r_1-r_i)^2)\exp\left(-\alpha_j(r_1-r_j)^2\right) = G_p\exp\left(-\alpha_p(r_1-r_p)^2\right)$$

- Where :

$$\alpha_p = \alpha_i + \alpha_j, \qquad r_p = \frac{\alpha_i r_i + \alpha_j r_j}{\alpha_p}, \qquad G_p = \exp(-\frac{\alpha_i\alpha_j(r_i - r_j)^2}{\alpha_p})$$

- We can use this theorem to transform our integral:

$$[p|q] = \int \frac{1}{r_1 - r_2}$$

$$\times {x_{1i}}^{n_i}{y_{1i}}^{l_i}{z_{1i}}^{m_i}{x_{1j}}^{n_j}{y_{1j}}^{l_j}{z_{1j}}^{m_j}\,G_p\exp\left(-\alpha_p(r_1-r_p)^2\right)$$

$$\times {x_{2s}}^{n_s}{y_{2s}}^{l_s}{z_{2s}}^{m_s}{x_{2t}}^{n_t}{y_{2t}}^{l_t}{z_{2t}}^{m_t}G_q\exp\left(-\alpha_q(r_2-r_q)^2\right)dr_1dr_2$$

- Here we get p from i and j, and q from s and t. So we get a two dimensional grid. This 2-D grid is suitable for parallelization and vectorization.

Recursion Relation Method

- There are three recursion schemes to calculate the integral:
  - The Dupuis-Rys-King (DRK) scheme, the Obara-Saika (OS) scheme and the McMurchie-Davidson (MD) scheme.
  - These 3 schemes have different recursion relations, but are mathematically equivalent.
- We use MD scheme, so the integral become the linear combination of several auxiliary functions.

$$[p|q] = G_p G_q \sum_{n_p}^{n_i+n_j} \sum_{l_p}^{l_i+l_j} \sum_{m_p}^{m_i+m_j} \sum_{n_q}^{n_s+n_t} \sum_{l_q}^{l_s+l_t} \sum_{m_q}^{m_s+m_t} d_{ij}^{x}(n_p) d_{ij}^{y}(l_p) d_{ij}^{z}(m_p)$$
$$\times d_{st}^{x}(n_q) d_{st}^{y}(l_q) d_{st}^{z}(m_q)$$
$$\times \gamma (-1)^{n_q+l_q+m_q} R(n_p+n_q, l_p+l_q, m_q+m_p, 0)$$

- The coefficient $d_{ij}^{x}(n_p)$ is generated by recursion relations:

$$d_{ij}^{x}(n_p, n_i+1, n_j) = \frac{1}{2\alpha_p} d_{ij}^{x}(n_p-1, n_i, n_j) + (x_p - x_i) d_{ij}^{x}(n_p, n_i, n_j) + (n_p+1) d_{ij}^{x}(n_p+1, n_i, n_j)$$

$$d_{ij}^{x}(0,0,0) = 1$$

Recursion Relation Method

- Also the auxiliary function $R(n, l, m, j)$ can be calculated by the recursion relations:

$$R(n+1, l, m, j) = x_T R(n, l, m, j+1) + nR(n-1, l, m, j)$$
$$R(n, l+1, m, j) = y_T R(n, l, m, j+1) + lR(n, l-1, m, j)$$
$$R(n, l, m+1, j) = z_T R(n, l, m, j+1) + mR(n, l, m-1, j)$$

- Where:

$$R(0,0,0,j) = (-2\alpha_T)^j F_j(T)$$
$$T = \alpha_T(x_T^2 + y_T^2 + z_T^2),$$
$$x_T = x_p - x_q, y_T = y_p - y_q, z_T = z_p - z_q,$$
$$\alpha_T = \alpha_p \alpha_q / (\alpha_p + \alpha_q)$$

- Finally $F_j(T)$ is a lower incomplete gamma function:

$$F_j(T) = \int_0^1 u^{2j} \exp(-Tu^2) du$$

Lower Incomplete Gamma Function

- Lower incomplete gamma function:

$$F_j(T) = \int_0^1 u^{2j} \exp(-Tu^2) du$$

- For 0≤T≤12:
  - Interpolation method (Taylor expansion):

$$F_j(T) = \sum_{k=0}^{6} F_{j+k}(T^*)(T^* - T)^k / k!$$

  - Series method:

$$F_j(T) = \frac{1}{2} \sum_{k=0}^{15+4T} \frac{(-1)^k T^k}{(j + k + 0.5)k!}$$

- For T>12:
  - Downward recursion relation:

$$F_j(T) = [2TF_{j+1}(T) + \exp(-T)]/(2j + 1)$$

$$F_0(T) = \frac{\pi^{1/2}}{2T^{1/2}} - \int_1^\infty \exp(-Tu^2) du$$

Mathematics Summary

- Given serial of N $\varphi(r)$ functions, the total number of ERI calculation is N^4.
- All primitive integral calculations are independent.
- Gaussian product theorem can help get a 2-D grid.
- For MD scheme, we have 3 recursion relations.
- For incomplete gamma function, interpolation method vs. series method.

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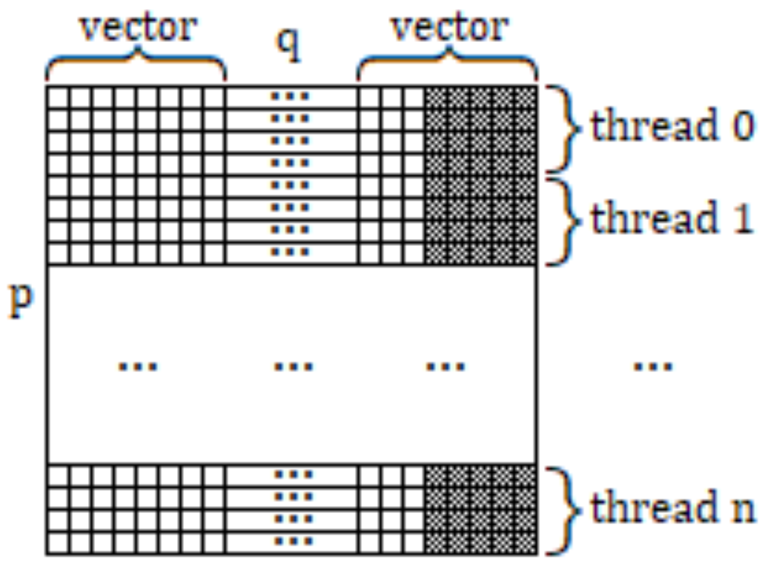
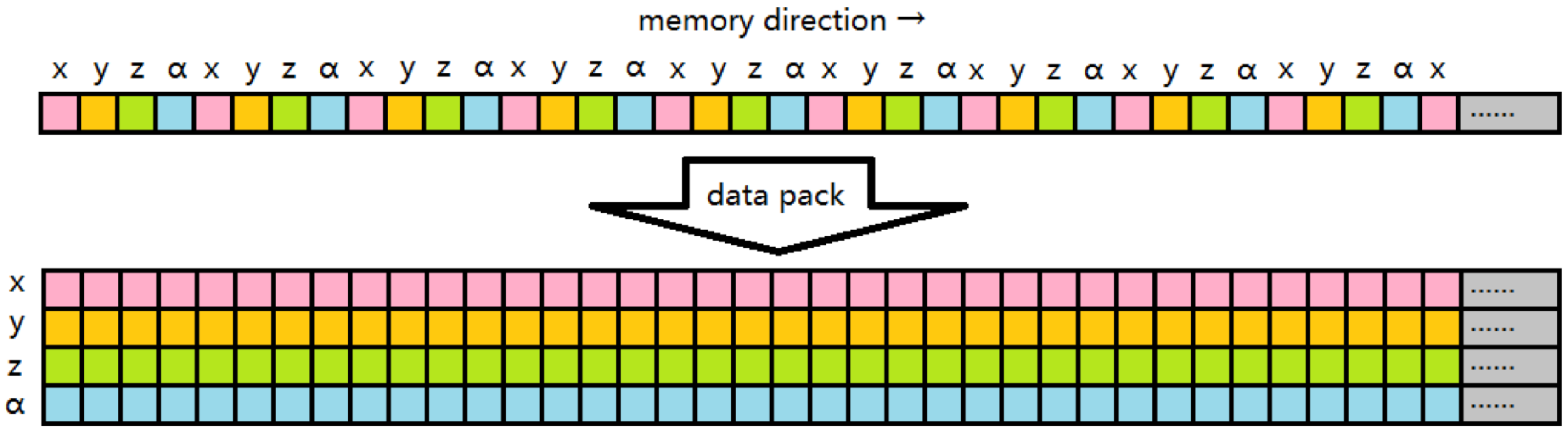
Parallelization and Vectorization Schedule

- This picture shows the 2-D grid:
  - Small block represents a integral task;
  - Date repacked and aligned to 64bit;
  - Vectorization along the q direction;
  - Thread parallelization along the p direction.

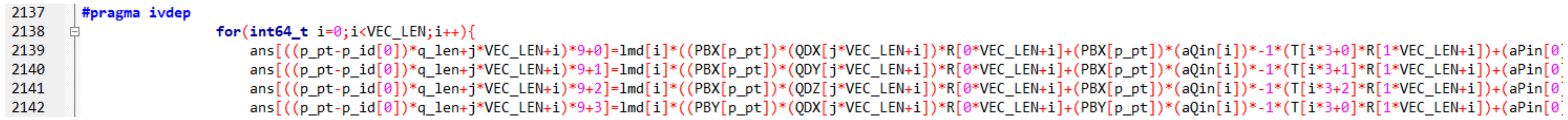




memory direction →
x y z α x y z α x y z α x y z α x y z α x y z α x y z α x y z α x y z α x
......
data pack
x
y
z
α

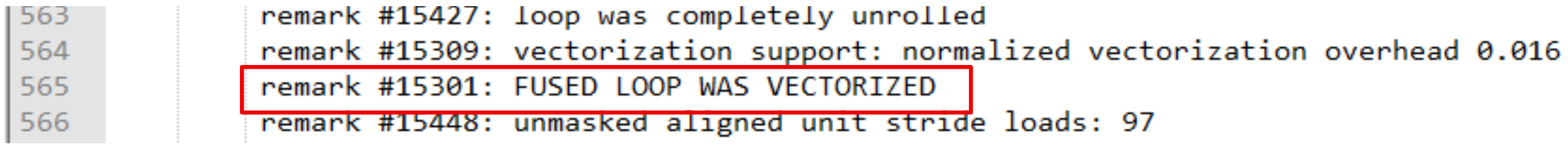
Vectorization for Recursion Relations

- A loops cannot be vectorized if a function is called in the loop.
- Inline method cannot be used for recursive functions.
- How to vectorize the recursion relations? Transform into loop?
- As the recursion relations are too complex, we decided to expand the calculation formula directly.
- We developed a program to automatically expand the formula and generate the codes:



```
#pragma ivdep
                for(int64_t i=0;i<VEC_LEN;i++){
                    ans[((p_pt-p_id[0])*q_len+j*VEC_LEN+i)*9+0]=lmd[i]*((PBX[p_pt])*(QDX[j*VEC_LEN+i])*R[0*VEC_LEN+i]+(PBX[p_pt])*(aQin[i])*-1*(T[i*3+0]*R[1*VEC_LEN+i])+(aPin[0
                    ans[((p_pt-p_id[0])*q_len+j*VEC_LEN+i)*9+1]=lmd[i]*((PBX[p_pt])*(QDY[j*VEC_LEN+i])*R[0*VEC_LEN+i]+(PBX[p_pt])*(aQin[i])*-1*(T[i*3+1]*R[1*VEC_LEN+i])+(aPin[0
                    ans[((p_pt-p_id[0])*q_len+j*VEC_LEN+i)*9+2]=lmd[i]*((PBX[p_pt])*(QDZ[j*VEC_LEN+i])*R[0*VEC_LEN+i]+(PBX[p_pt])*(aQin[i])*-1*(T[i*3+2]*R[1*VEC_LEN+i])+(aPin[0
                    ans[((p_pt-p_id[0])*q_len+j*VEC_LEN+i)*9+3]=lmd[i]*((PBY[p_pt])*(QDX[j*VEC_LEN+i])*R[0*VEC_LEN+i]+(PBY[p_pt])*(aQin[i])*-1*(T[i*3+0]*R[1*VEC_LEN+i])+(aPin[0
```

- And the compiler report shows the loop was vectorized:



```
remark #15427: loop was completely unrolled
remark #15309: vectorization support: normalized vectorization overhead 0.016
remark #15301: FUSED LOOP WAS VECTORIZED
remark #15448: unmasked aligned unit stride loads: 97
```

Interpolation Method vs. Series Method

- As I mentioned before, lower incomplete gamma function can be calculated by two method:
  - Interpolation method (Taylor expansion):

$$F_j(T) = \sum_{k=0}^{6} F_{j+k}(T^*)(T^* - T)^k / k!$$

  - Series method:

$$F_j(T) = \frac{1}{2} \sum_{k=0}^{15+4T} \frac{(-1)^k T^k}{(j + k + 0.5)k!}$$

- For interpolation method, $F_{j+k}(T^*)$ is previously calculated and stored in memory for $T^* = 0, 0.1, 0.2 \ \ldots 12$ and j from 0 to 16. So it has 7 memory load instructions for each $F_j(T)$.
- For series method, it`s just calculations.

Code structure

```
Loop i:
    Loop j:
        Get p in aligned memory;
    End loop j;
End loop i;

Parallel loop p:
    Loop q/(vector length):
        Vector loop:
            Get R(0,0,0,j) for j=0~L from $F_j(T)$;
            Integral calculation [p|q] with expanded codes;
        end vector loop;
    End loop q;
End loop p;
```

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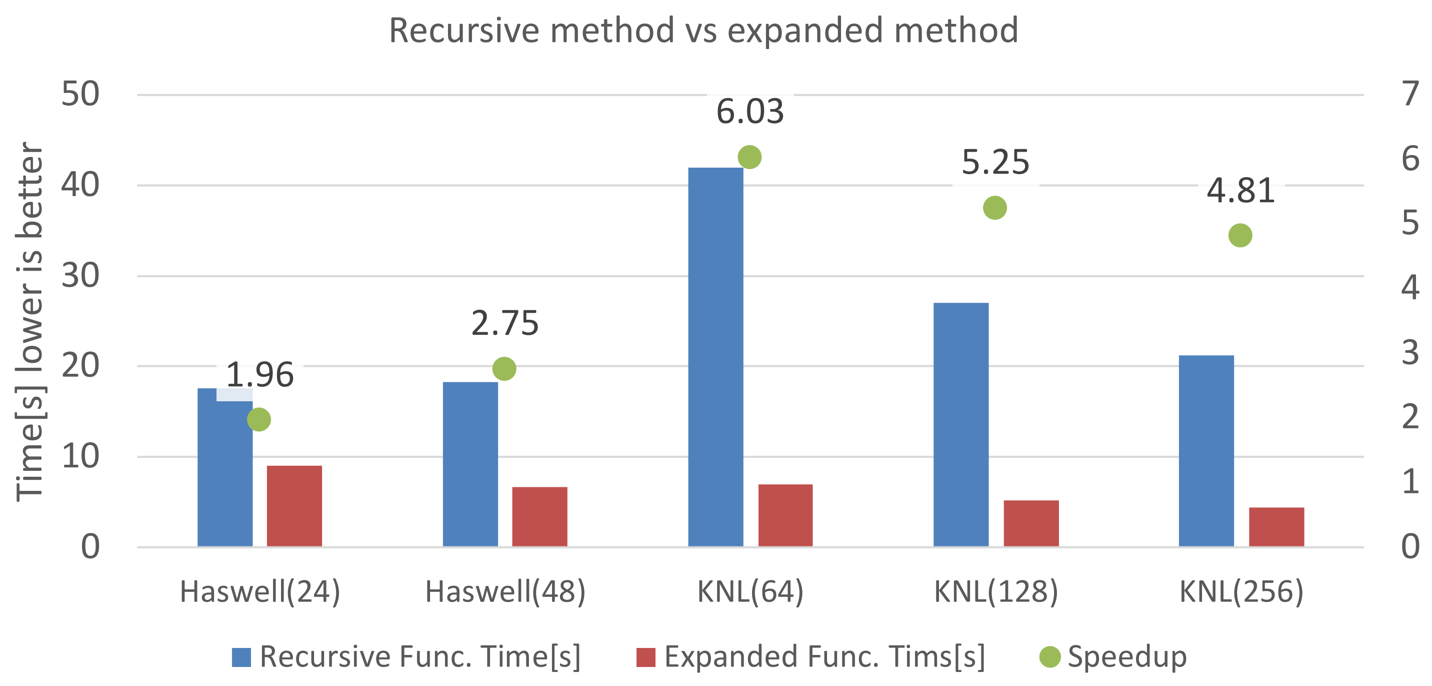
Platform and Benchmark Molecules

- Haswell platform:
  - 2 × Intel Xeon E5-2680v3 12 cores @ 2.50GHz 120W
  - 2 × 256-bit Vector Processing Unit per core
  - 0.96GFLOPS
- KNL platform:
  - Intel Xeon Phi 7210 64 cores @ 1.30GHz 215W
  - 2 × 512-bit Vector Processing Unit per core
  - 2.66GFLOPS
- Benchmark Molecules:

No.	Molecule	No. of atoms	No. of basis functions
1	Caffeine	24	146
2	Cocaine	43	240
3	Protein 1	71	408
4	Taxol	110	647
5	Protein 2	145	815
6	Valinomycin	168	882

Recursive vs. Expanded

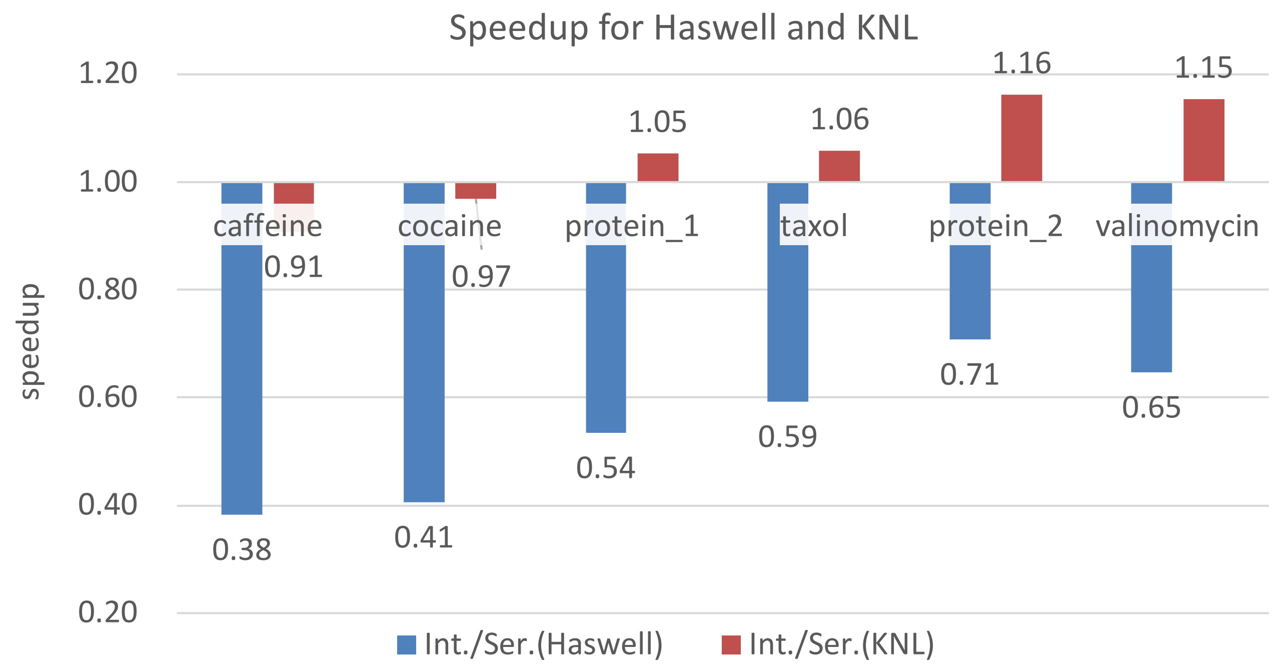
- We choose the $F_j(T)$ downward recursion relation (3rd) to show the different performances between recursive function and expanded function:



- As the expanded function can be vectorized and no function call, it performs better on both platform.

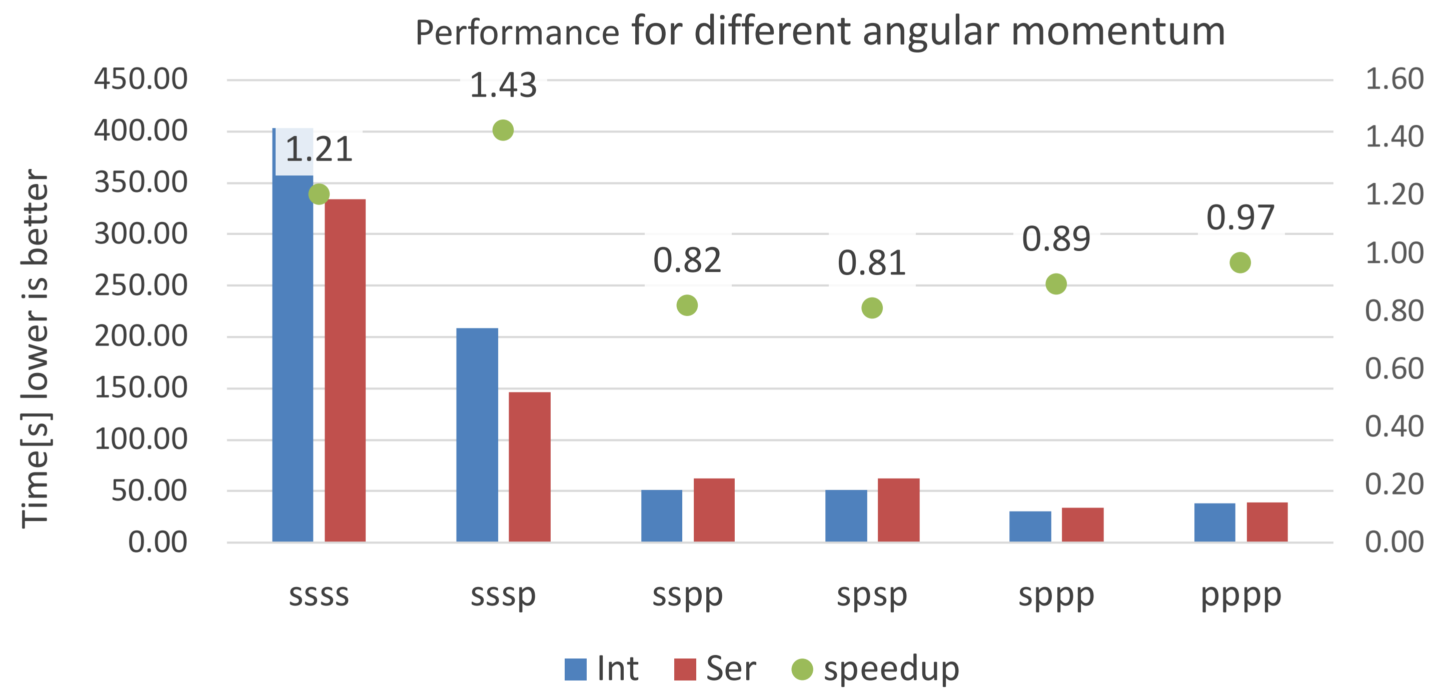
Interpolation vs. Series

- We implemented both interpolation method and series method for $F_j(T)$ calculation, and tested on both platform:
  - Interpolation method performs better on Haswell;
  - Series method performs better on KNL;



Interpolation vs. Series

- If we check the series method performance for different angular momentum L on KNL:
  - Series method performs better when angular momentum L is small.



Vectorization

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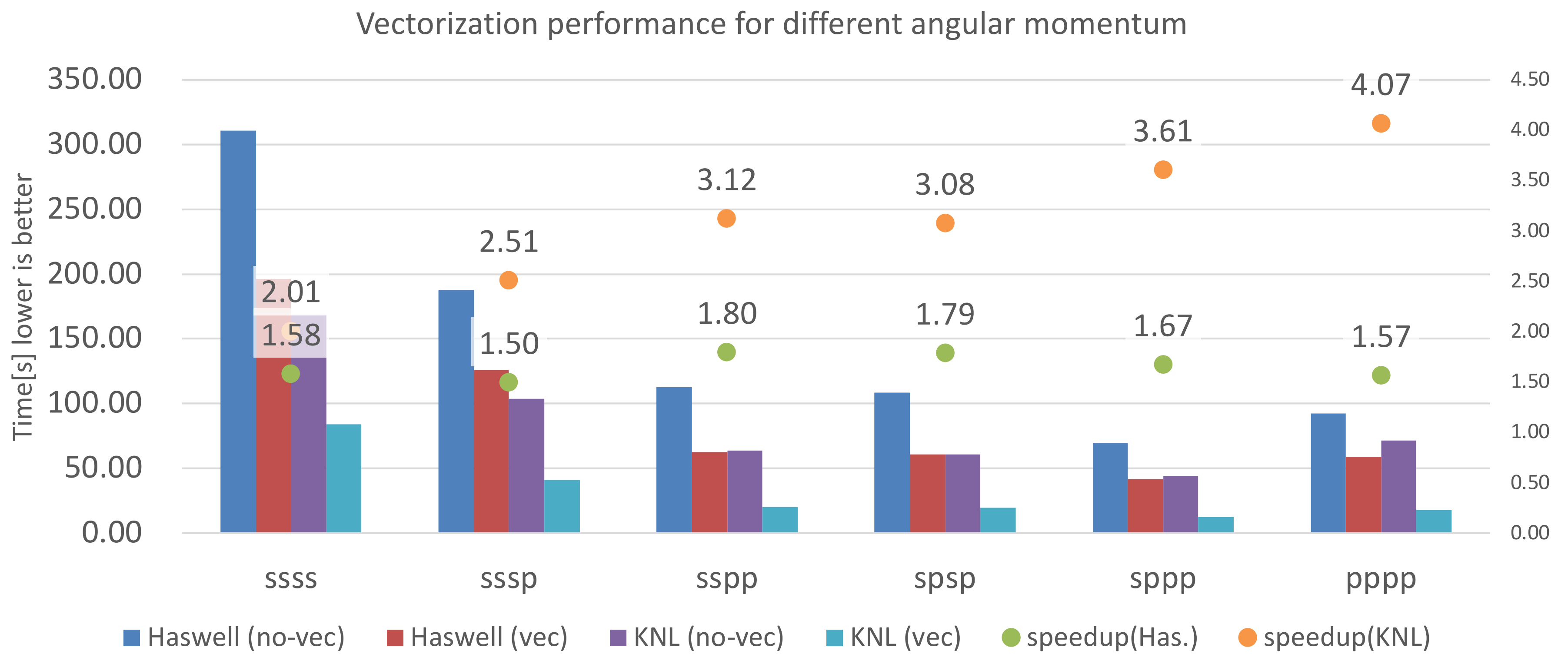
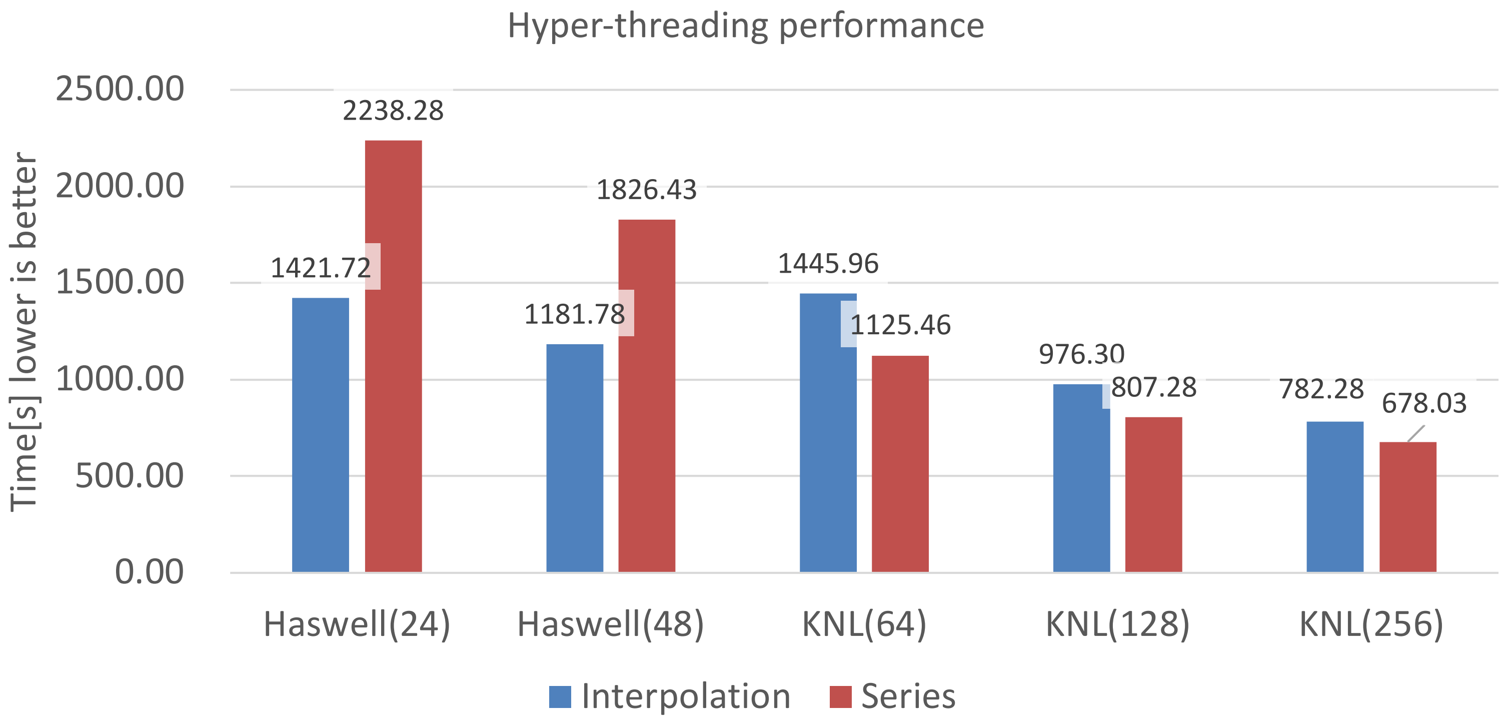
- We compiled our codes with –vec and –no-vec compile options to see how well our vectorization method performed:



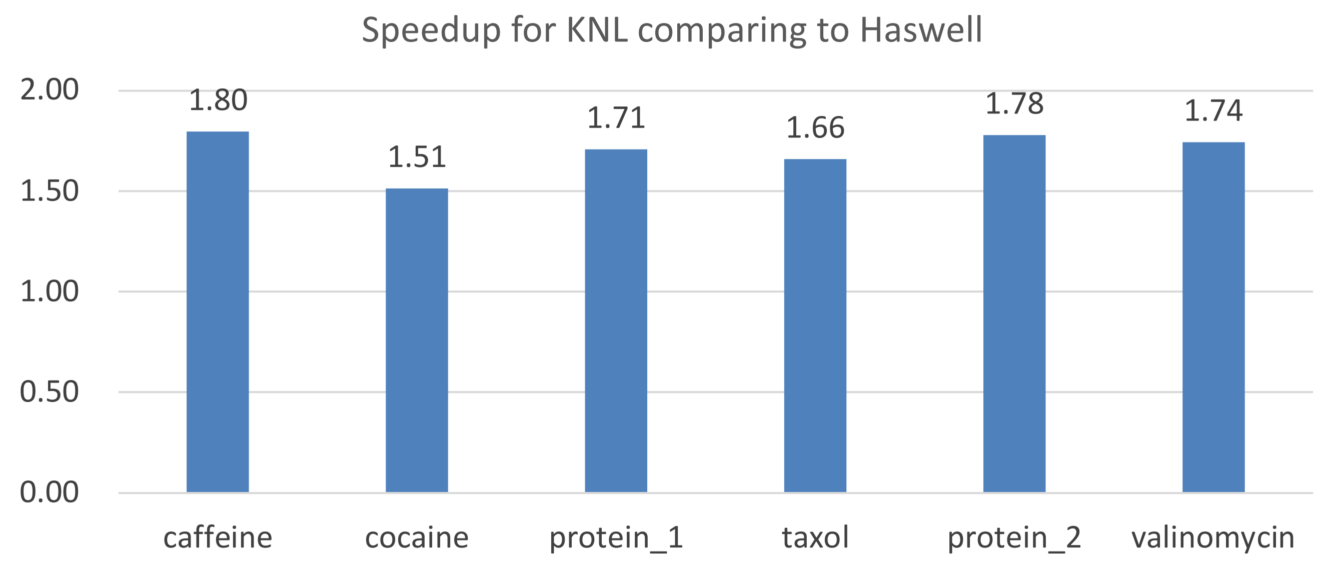
Hyper-threading

- We also tested the hyper-threading performance:
  - Haswell support 2 thread per core
  - KNL support up to 4 thread per core
  - KMP_AFFINITY=scatter



Over All KNL Speedup

- By applying all these optimization methods, we have the final result:
  - We get up to 1.80 performance speed up on KNL comparing to Haswell.
  - Average speedup is 1.70.



Conclusion

- We developed a parallelization and vectorization scheme for ERI.
- We developed a program to automatically expand recursion relation formula and generate vectorizable codes. Expanded codes performed pretty well both on Haswell and KNL.
- We found interpolation method performed better on Haswell but series method performed better on KNL.
- Over all, we get up to 1.80 speedup on KNL comparing to Haswell.

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Thank you for your attention！

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