High-Performance X-Ray Scattering Data Analysis

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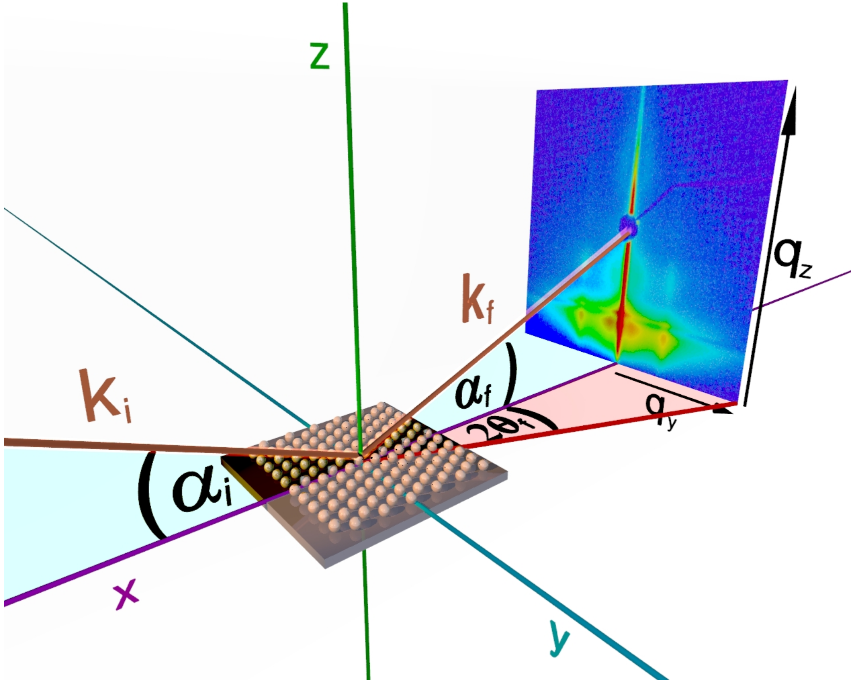
Background

- **HipGISAXS:**
  a massively-parallel
  high-performance
  grazing incidence small angle
  X-ray scattering data analysis
  software.

- Written in **C++** with
  MPI + OpenMP [+ CUDA.]

- **Double-precision complex** number computations.



An Example Kernel

```
for(int z = 0; z < nqz; ++ z) {                                    // O(10^6)
    int y = z % nqy;
    vector3c_t mq = rotate(qx[y], qy[y], qz[z], rot);
    complex_t qpar = sqrt(mq[0] * mq[0] + mq[1] * mq[1]);

    ... more computations ...

    complex_t temp_ff(0.0, 0.0);
    for(int i_r = 0; i_r < rsize; ++ i_r) {                        //  O(1) - O(10)
        for(int i_h = 0; i_h < hsize; ++ i_h) {                    //  O(1) - O(10)

            ... more computations ...

            complex_t expo_val = exp(0.5 * mq[3] * h[i_h]);
            complex_t sinc_val = sinc(0.5 * mq[3] * h[i_h]);
            complex_t bess_val = cbessj(qpar * r[i_r], 1) / (qpar * r[i_r]);
            temp_ff += sinc_val * expo_val * bess_val;
        }
    }

    ... more computations ...

    complex_t temp2 = exp(temp1);
    ff[z] = temp_ff * temp2;
}
```

Optimizing for Intel Processors: Platforms for Analysis

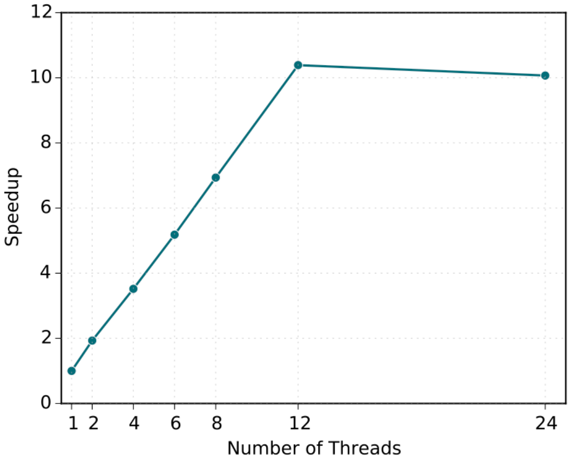
- **Edison** (Cray XC30) @ NERSC:
  - Intel Ivy Bridge (Xeon E5-2695). 12 cores.

- **Babbage** @ NERSC:
  - Intel Xeon Phi (KNC). 60 cores.

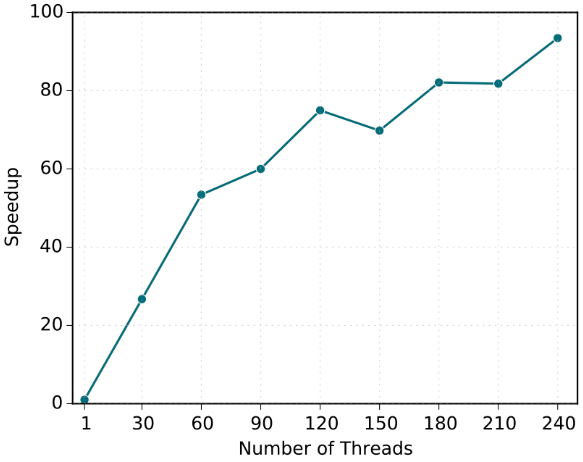
Optimizing for Intel Processors: Threading

- Mostly *embarrassingly-parallel* computations.
- Primary performance analysis tools used:
  - *Intel VTune, TAU, PAPI.*
- Effective threading using **OpenMP**:

On **Edison**:
(Ivy Bridge)



On **Babbage**:
(MIC/KNC)



Kernel Vectorization: Attempt 1

- **Compiler-based auto-vectorization.** (Intel compiler 15.0.)
- **Requirements for auto-vectorization:**
  - Loop should be single-block, typically without branches/jumps.
  - Loop must be countable.
  - No backward loop-carried dependencies.
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- **Pragmas and explicit directives failed.**

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- **VML mode LA** (*Low Accuracy, 4 ulp.*)
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- **VML mode EP** (*Enhanced Performance, 50% bits accurate.*)
  - ➢ *IvyBridge:* Time = **0.50x** base [speedup = **1.98**], # instructions = **0.61x** base.
  - ➢ *MIC:* Time = **0.086x** base [speedup = **11.64**].

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inline avx_m256c_t avx_mul_ccp(avx_m256c_t a, avx_m256c_t b) {
    avx_m256c_t v;
    avx_m256_t temp1 = _mm256_mul_pd(a.real, b.real);
    avx_m256_t temp2 = _mm256_mul_pd(a.imag, b.imag);
    avx_m256_t temp3 = _mm256_mul_pd(a.real, b.imag);
    avx_m256_t temp4 = _mm256_mul_pd(a.imag, b.real);
    v.real = _mm256_sub_pd(temp1, temp2);
    v.imag = _mm256_add_pd(temp3, temp4);
    return v;
}
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    v.real = _mm256_sub_pd(temp1, temp2);
    v.imag = _mm256_add_pd(temp3, temp4);
    return v;
}
```

- **Performance:**
  - ➢ Time = **0.35x** base [speedup = **2.86**], # instructions = **0.28x** base.

Conclusions and Insights

- **Auto-vectorization does not always work.**
- **Intrinsics are best for DP/complex computations.**
  - Provide most flexibility in achieving higher performance for *non-typical* computes.
- **Biggest surprises: Intel MKL performance, e.g.** **`v?Exp()`**
  - DP complex, average MKL time = **0.93x** base [speedup = **1.08**]
  - DP real, average MKL time = **0.53x** base [speedup = **1.87**]
  - SP complex, average MKL time = **0.34x** base [speedup = **2.97**]
  - SP real, average MKL time = **0.25x** base [speedup = **4.07**]
- **Would be great if efficient implementations of special functions like Bessel, Sinc were available.**
- **Already taking Intel's help.**

Acknowledgements

- This work was performed as part of the **"Lawrence Berkeley National Lab Intel Parallel Computing Center."**
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- Inputs/suggestions were obtained from Intel folks: **Marius Cornea, Jingwei Zhang, CJ Newburn, Hideki Saito.**