Parallelization of Atomic Image Reconstruction from X-ray Fluorescence Holograms with XcalableMP

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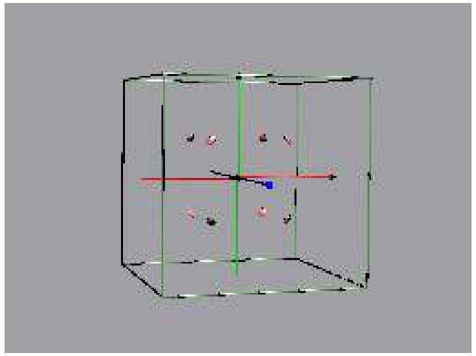
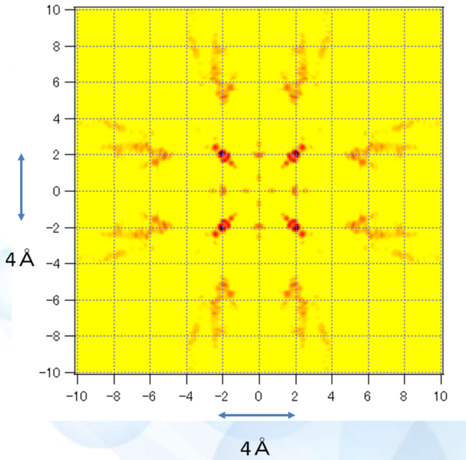
Outline

- What is “X-ray Fluorescence Holography” ?
- Parallelization of 3D atomic image reconstruction
- Evaluation on PC cluster
- Conclusion





Conventional techniques such as X-ray diffraction
→ Global structure analysis

Our Approach

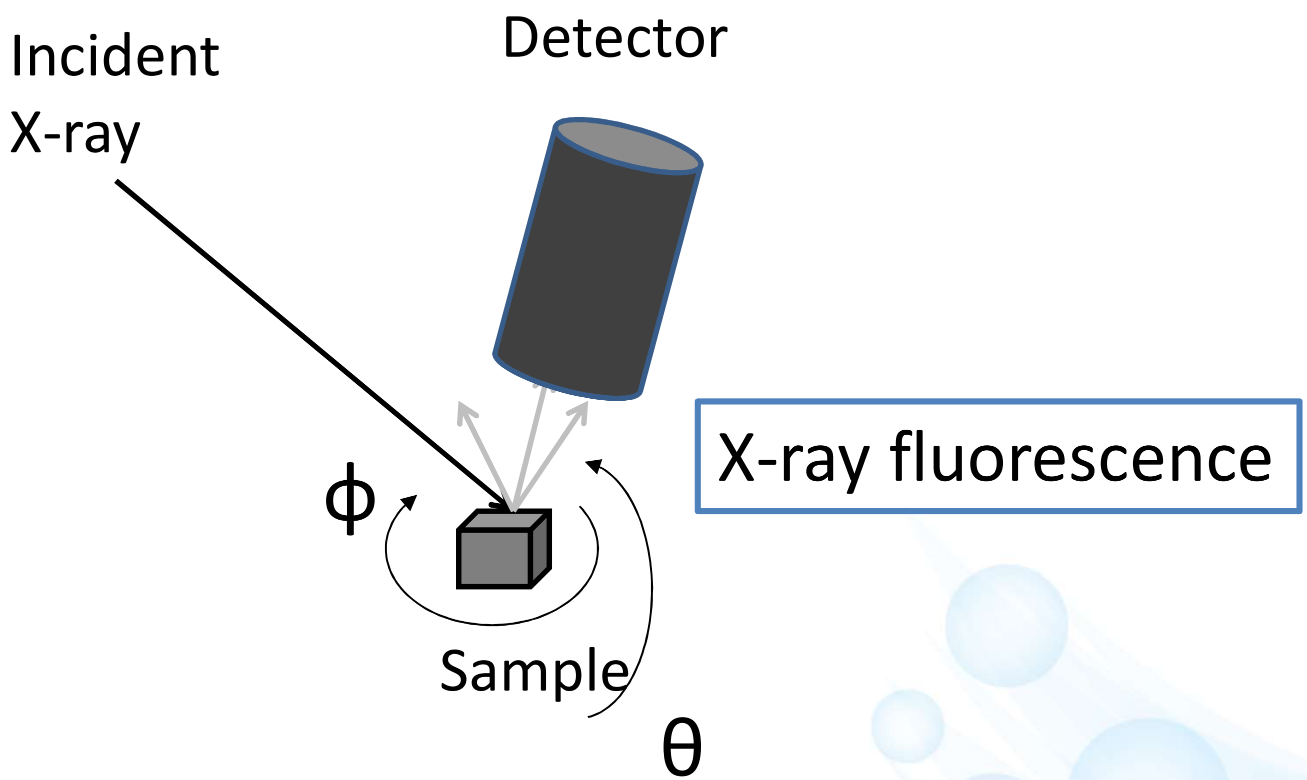
From http://www.3d-activesite.jp

In many functional materials, the local structure of the "**dopant**," "**hetero-interface**," and "**nanomaterial**," i.e., the "**Active-Sites**" in the parent material play a vital role in the functional expression of the material

3D Atomic Resolution Imaging

- **Fluorescent X-rays** and Photoelectron **Holography**
- Surface/Interface Holography
- Nano-structure Imaging

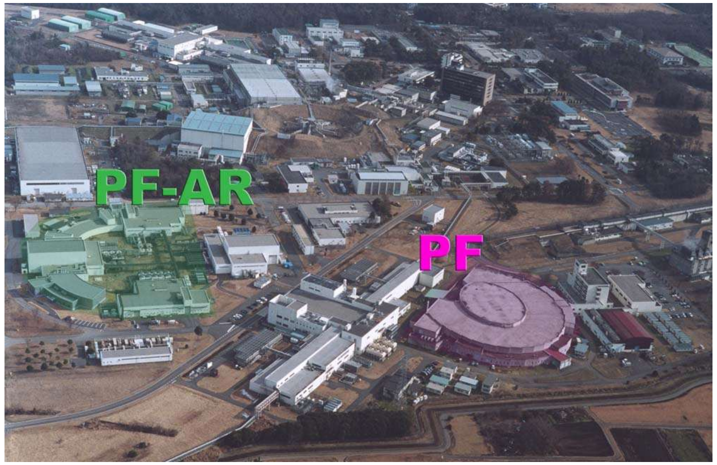
Experiment : Inverse Mode of X-ray Fluorescence Holography



Intensity of X-ray fluorescence is measured
while rotating samples

3D ACTIVE SITE SCIENCE

Synchrotron radiation facilities



Spring-8
http://www.spring8.or.jp

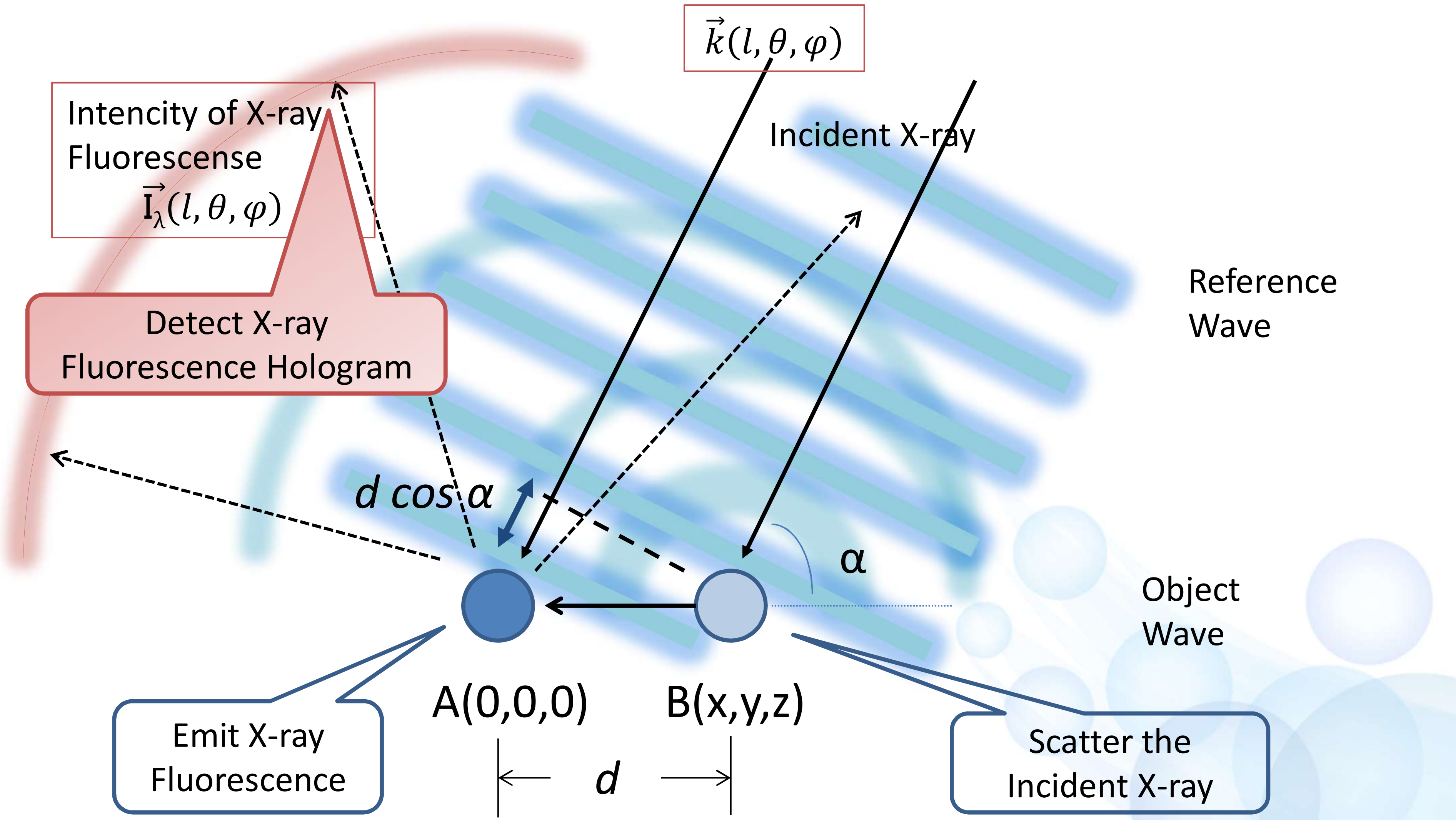
Photon Factory,
High energy accelerator
http://www2.kek.jp/imss/pf/

KEK 大学共同利用機関法人 高エネルギー加速器研究機構

SPring-8

放射光科学研究施設 Photon Factory

Principle of Inverse Mode



Analysis Procedure of Atomic Image Reconstruction from X-ray Fluorescence Holograms

Holograms obtained by Experiment

↓

Removal of background waves

↓

Completion of sphere data

↓

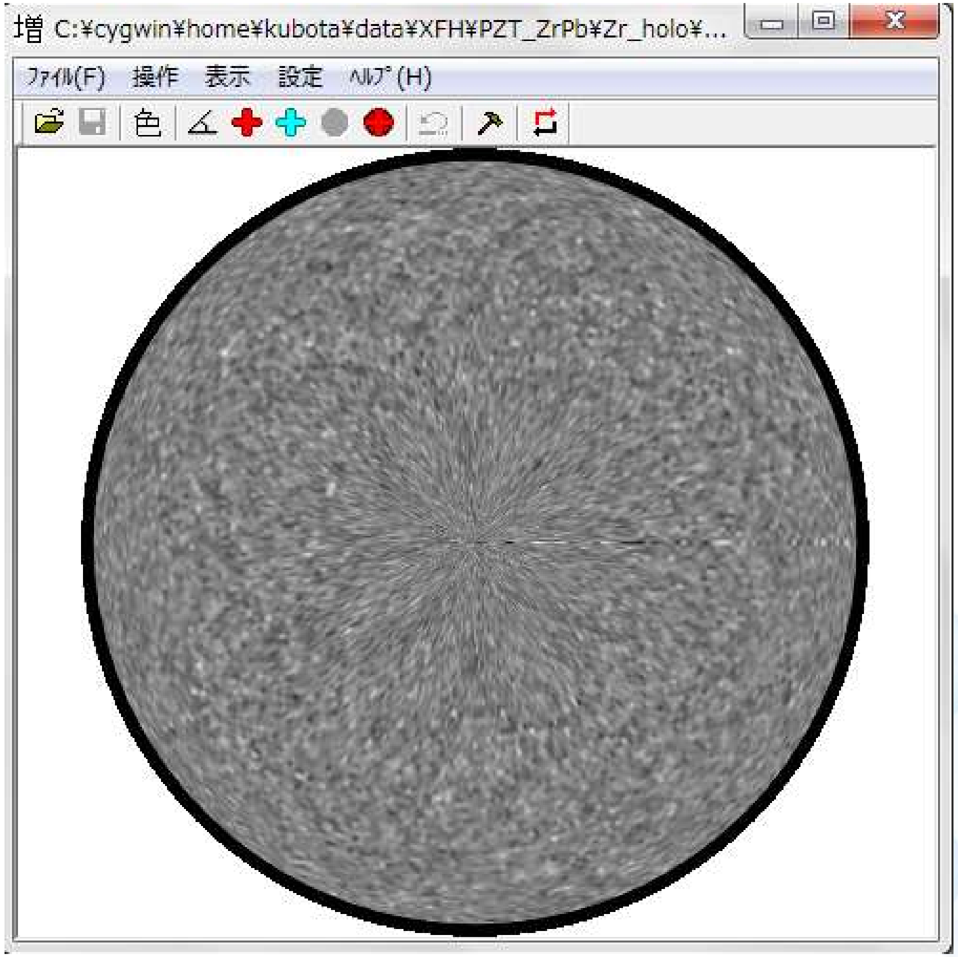
Reconstruction of atomic images (same as discrete Fourier transform)

Long time required for Reconstruction on computer

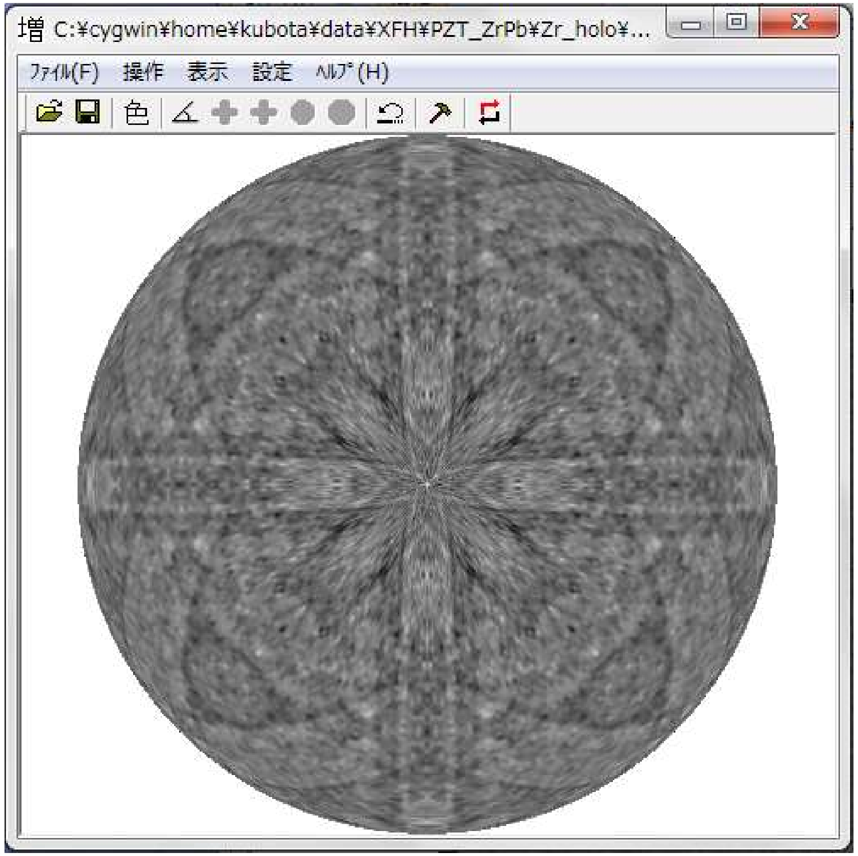
↓

Performance improvement needed

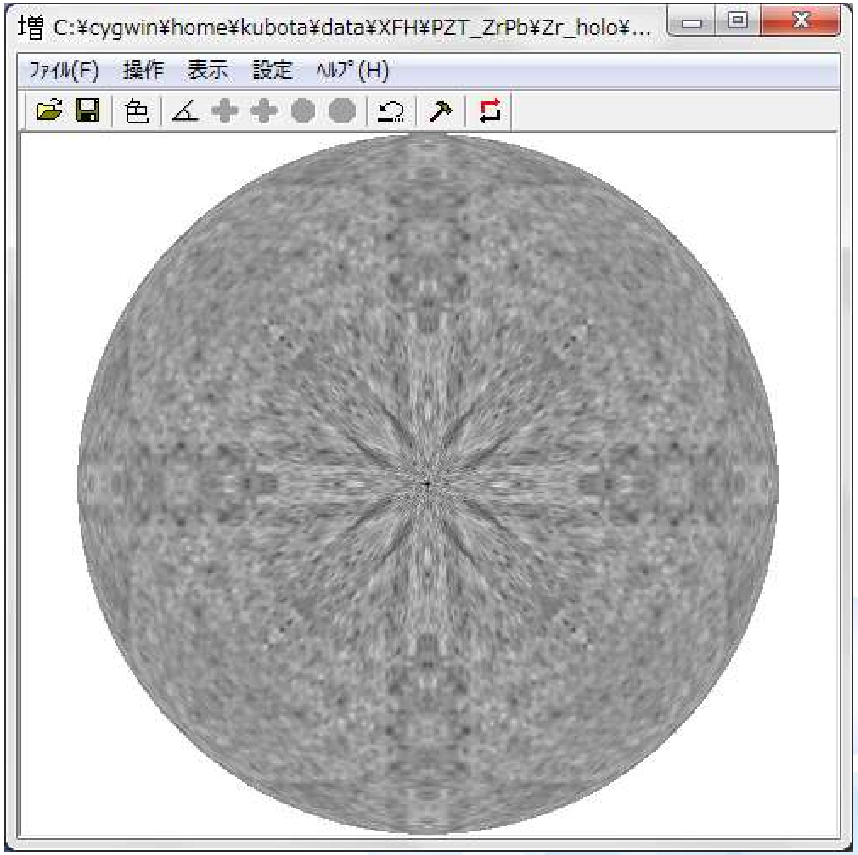
A Hologram after removel of background waves



Holograms after completion of sphere data

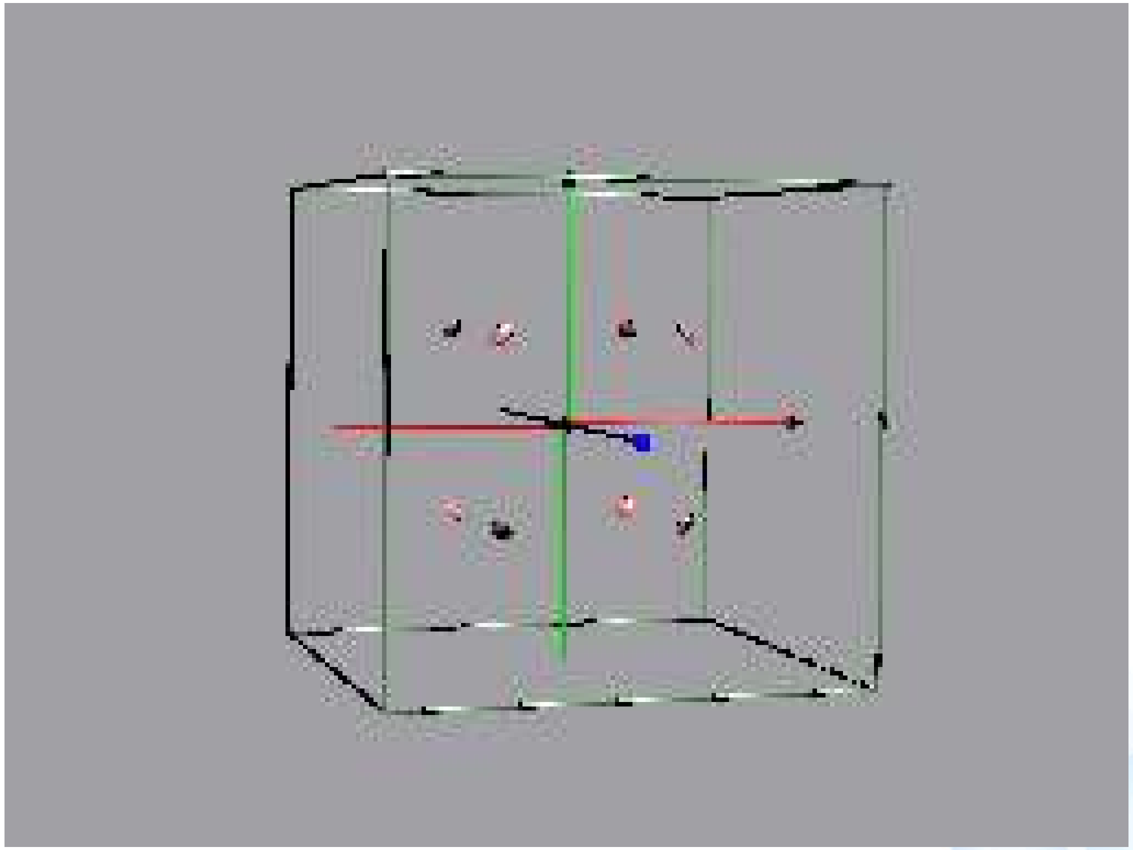


18500 eV

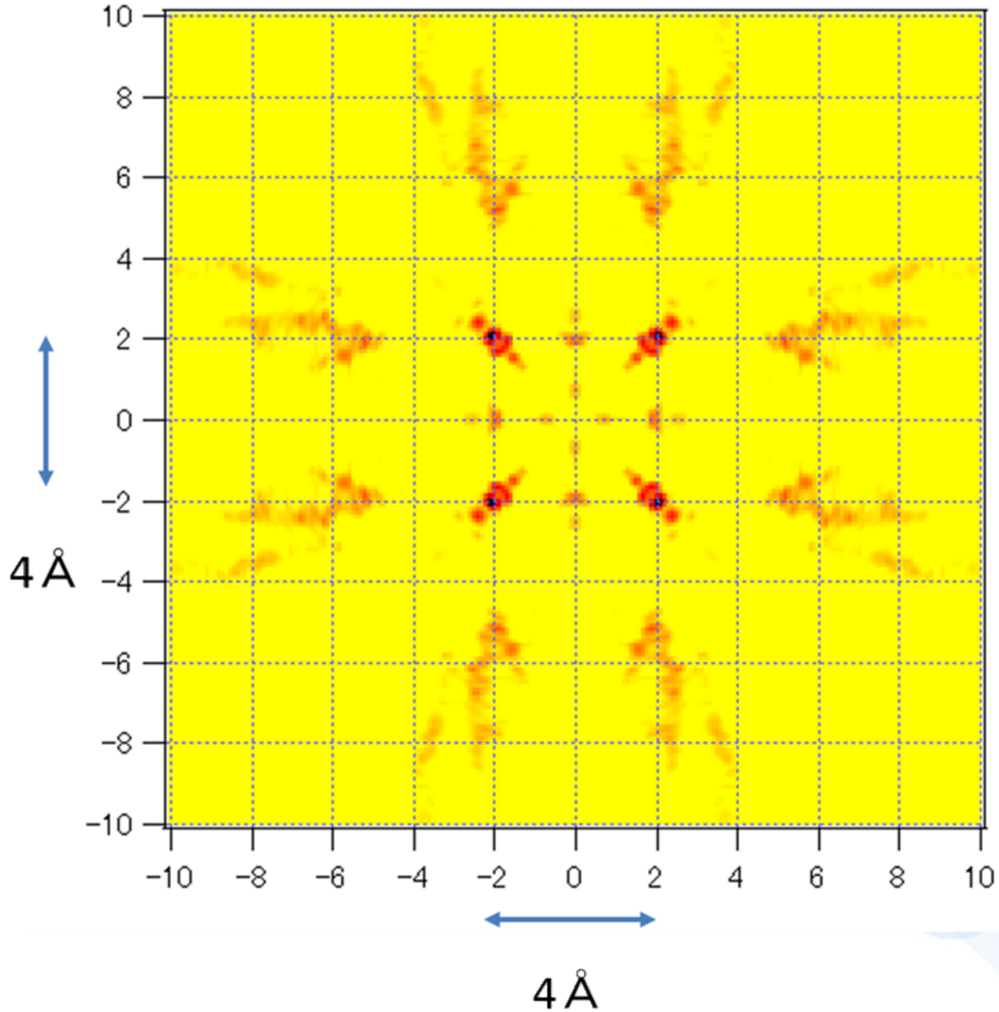


23500 eV

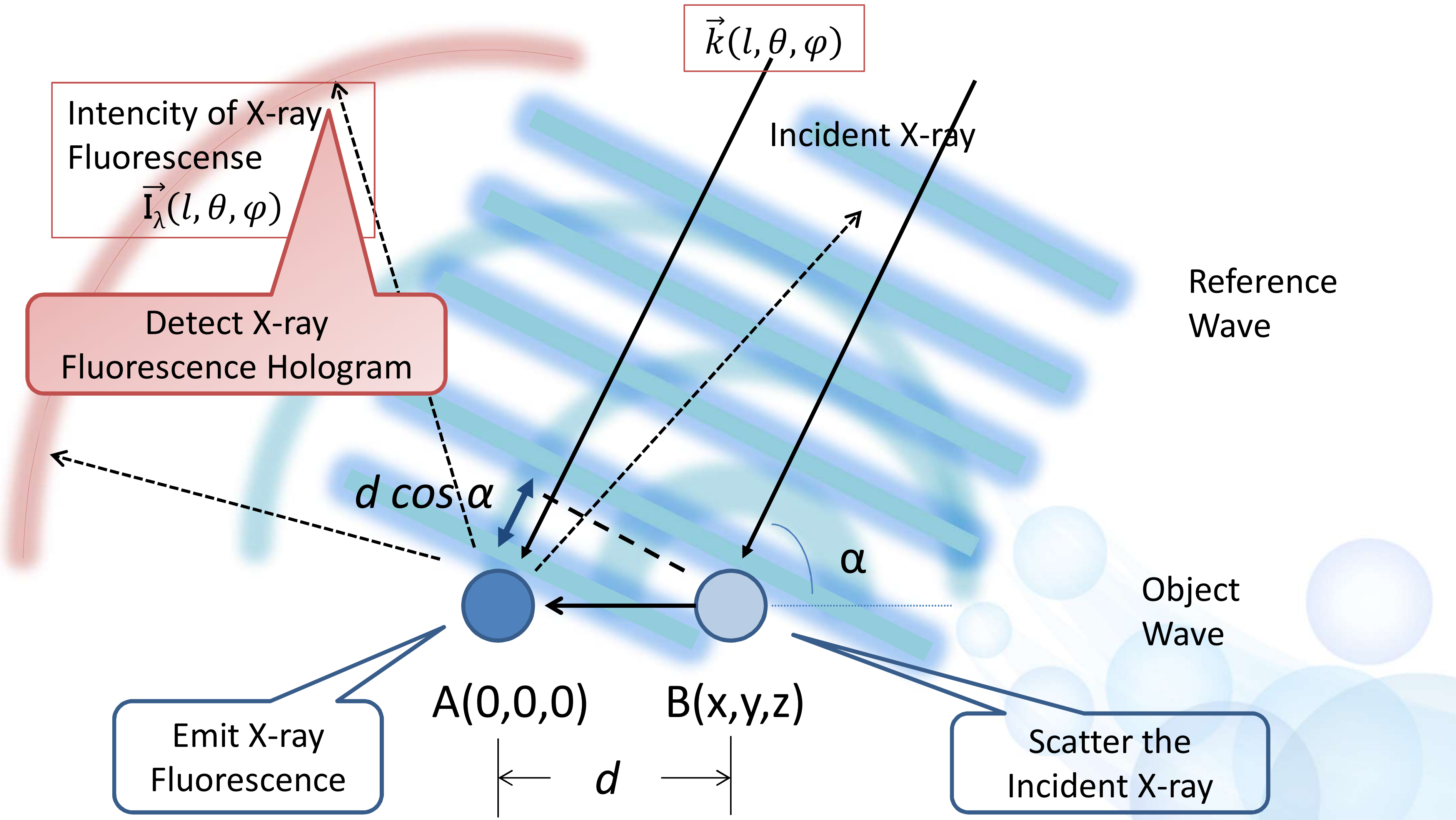
An example 3D reconstructed image



An example of 2D reconstructed image (z=2.0)



Principle of Inverse Mode



3D Atomic Image Reconstruction by Discrete Fourier Transform

3D ACTIVE SITE SCIENCE

Detection of X-ray Fluorescence Hologram

Position on the sphere l distance apart from sample : $\vec{k}(l,\theta,\varphi)$

Intensity of X-ray fluorescence : $\vec{I_\lambda}(\theta,\varphi)$

Position of atom A : O$(0,0,0)$

Position of atom B : $\vec{r}(x,y,z)$

Caluculation of image χ at $\vec{r}(x,y,z)$

Parallelizable for $X,\ Y,\ Z$

Sum for θ,φ,λ

$$\chi(x,y,z) = -\sum_{\theta}\sum_{\varphi}\sum_{\lambda} \mathrm{I}_\lambda(\theta,\varphi)\exp\left(i2\pi\left(|\vec{r}| - \vec{k}\,\vec{r}\right)/\lambda\right)\sin\theta\, w(\lambda)$$

Superimpose multiple holograms obtained by several input X-rays with different wave lengths λ → Reduction of ghost image

Parallelization of 3D Atomic Image Reconstruction

- Hard to apply FFT to Reconstruction(DFT)

  Input data on the polar coordinate system

  Output image on the rectangular coordinate system

- 2D atomic image reconstruction by OpenMP
- 3D atomic image reconstruction by hybrid parallelization of XcalableMP and OpenMP

Programming Languages / Libraries for Parallel Processing

High Level

Low Level

Distributed Memory

HPF

Go

Fortress

PGAS (XcalableMP, X10,Chapel, CAF,UPC)

MPI, PVM

socket

Shared Memory

OpenMP

TBB

OpenACC

OpenCL,CUDA

pthreads

shmem

Parallelization of 2D Atomic Image Reconstruction by OpenMP

- Loop interchange
  - Loop nest of $x,y,\theta,\varphi,\lambda$ to $\lambda,x,y,\theta,\varphi$
  - Expect
    - Improvement of cache hit ratio
    - SIMDization(such as Intel SSE) by increased number of iterations of the inner most loop
- Table look up of trigonometric function
  - Some calls of trigonometric functions are replaced with references of arrays calculated before entering loop
  - Some trigonometric calls remain in the kernel loop nest
- Parallelize x loop by OpenMP

Table Look-up of Trigonometric Function Calls

/* Trigonometric function calls in the loop*/

```
for(th=0;th<NTH;th++) {
  for(phi=0;phi<NPHI;phi++) {
    … cos(phi)
    … sin(phi)
  }
}
```

/* Save trigonometric function values */

```
for(phi=0;phi<NPHI;phi++) {
  ctab[phi]=cos(phi);
  stab[phi]=sin(phi);
}
```

/* Table loop-up in the loop */

```
for(th=0;th<NTH;th++) {
  for(phi=0;phi<NPHI;phi++) {
    … ctab[phi]
    … stab[th]
  }
}
```

Parallelization of 3D Atomic Image Reconstruction by XcalableMP

- The 6 nests of loop $\lambda,z,x,y,\theta,\varphi$
  - Z dimension is added to 2D reconstruction
- Table loop-up of trigonometric function calls
  - same as 2D reconstruction
- Parallelize z loop by XcalableMP

Data Declarations in XcalableMP

/* Input hologram in0 is duplicated in the all nodes */

```
double in0[NTH][NPHI];
```

/* Output image out1 is distributed among nodes */

```
double out1[NZ][NX][NY];
#pragma xmp nodes p(8)
#pragma xmp template t(NZ)
#pragma xmp distribute t(block) onto p
#pragma xmp align out1[z][*][*] with t(z)
```

/* Output image out2 is duplicatged in the all nodes */

```
double out2[NZ][NX][NY];
```

Parallelized Nest of Loops of 3D Atomic Image Reconstruction

```
for (lambda=0;lambda<NL;lambda++) {
#pragma xmp loop on t(z)
  for (z=0;z<NZ;z++) {
#pragma omp parallel for
    for (x=0;x<NX;x++) {
      for (y=0;y<NY;y++) {
        for (th=0;th<NTH;th++) {
          for (phi=0;phi<NPHI;phi++) {
            … ctab[phi]
            … stab[th]
            out1[z][x][y] = …
}}}}}}
```

Parallelize Z loop among nodes

Parallelize X loop on each node

File I/O and Aggregation of Data

/* Read input hologram in0 from file on the all nodes */

```
fread(in_file, in0,…);
```

```
…
/* Parallelized Kernel DFT Loop */
…
```

/* Aggregate distributed data out1 to out2 */

```
#pragma xmp gmove
out2[:][:][:] = out1[:][:][:];
```

/* Write atomic image out2 only on node 1 */

```
if(xmp_node_num()==1) {
  fwrite(out_file, out2,…);
}
```

Aggregation to avoid writing data to single file by multiple nodes

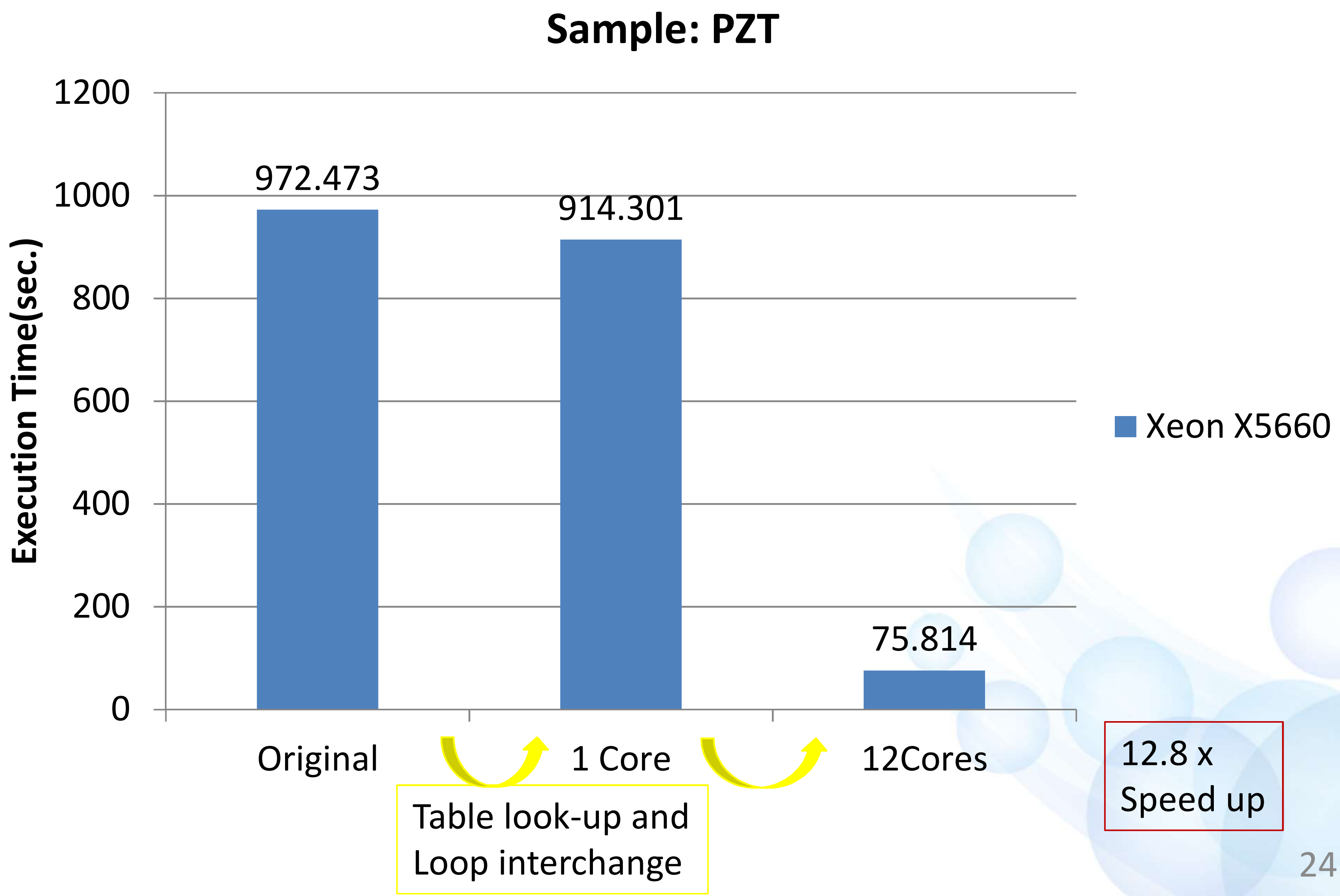
Performance Evaluation: I/O Data

- Input data file
  - Sample : PZT
  - Incident angle1 θ=1° ~ 179° , 1° resolution
  - Incident angle2 ϕ=0° ~ 359° , 1° resolution
  - Record measured intencity of X-ray fluorescence
  - Energy of incident X-ray
    - 18,500 eV – 23,500 eV
    - 250 eV step, 21 levels of energy
- Output data file
  - 2D atomic image: 192 × 192
  - 3D atomic image: 192 × 192 × 192
  - -9.6 Å ~ 9.6 Å , 0.1 Å resolution

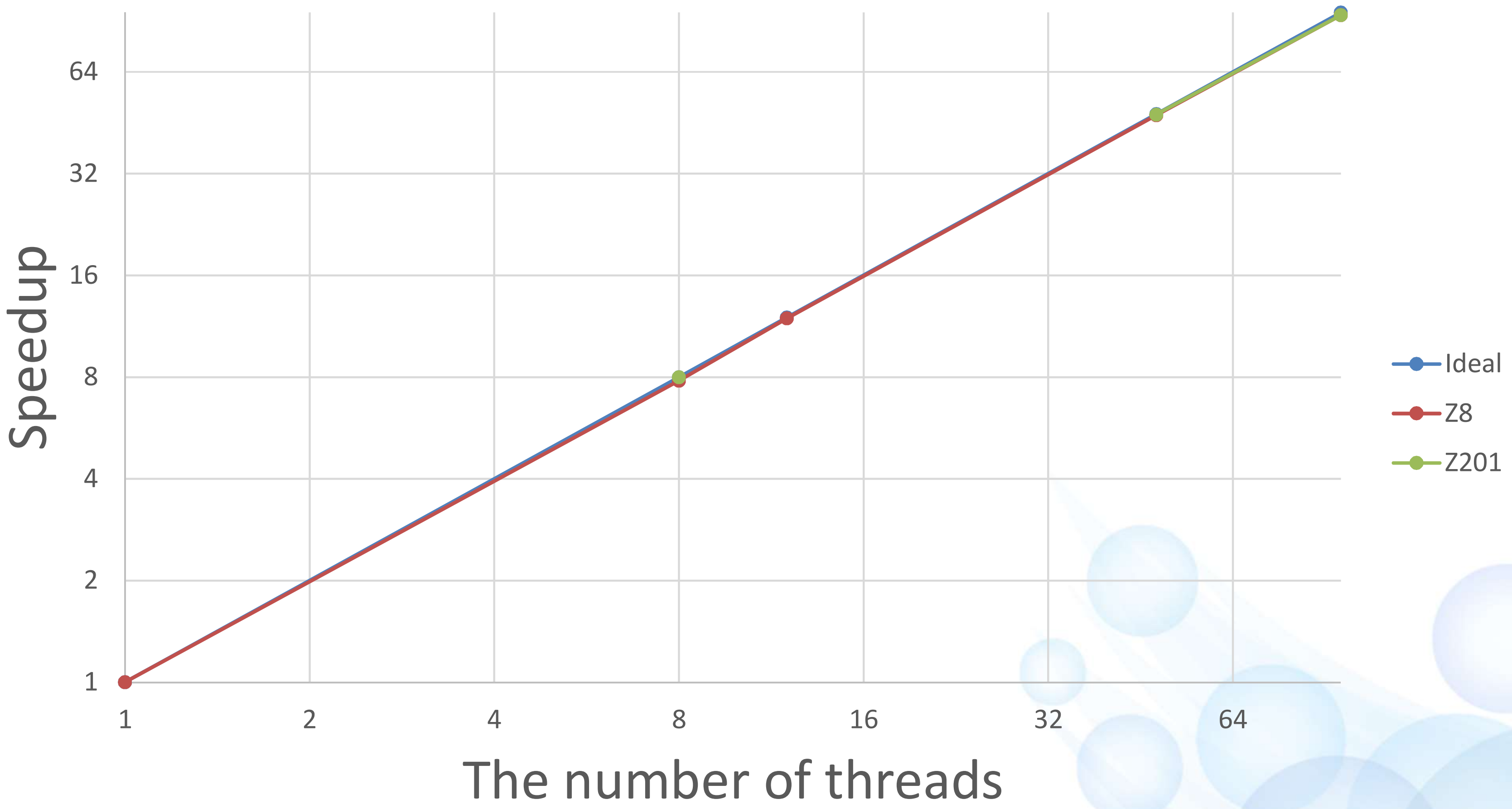
PC cluster used for reconstruction

	PC cluster
The number of nodes	8
The number of sockets / node	2
CPU	Xeon X5660 2.8GHz
The number of cores (threads)	6 cores (6threads, HT off)
The total number of cores	96
Cache size	L3:12MB
Inter-node network	4Gbps(InfiniBand DDR)
XcalableMP Compiler	1.2.2
Compiler, Optimization	Intel Compiler 18.0.1 –O3 -xHOST
OS	Linux (CentOS 6.3)

Results of 2D Atomic Image Reconstruction



Results of 3D Atomic Image Reconstruction



Parallelize loops with XMP and OpenMP

Break Down of Execution time

3D Image (NZ,NX,NY)=(**192**,192,192)

Total threads	(#Nodes × #Threads/Node)	Execution Time (sec.)	Speedup	File Input (sec.)	Aggregation (sec.)	File Output (sec.)
8	(8 × 1)	21,683.076	8.000	0.781	0.176	9.772
48	(8 × 6)	3,623.352	47.874	0.721	0.163	9.731
96	(8 × 12)	1,840.942	94.226	0.767	0.174	9.701

From 6 hours
To 30 min.

Estimated
2days with
single thread

3D Image (NZ,NX,NY)=(**8**,192,192)

Total thread	(#Nodes × #Threads/Node)	Execution Time (sec.)	Speedup	File Input (sec.)	Aggregation (sec.)	File Output (sec.)
1	(1 × 1)	7,214.325	1.000	0.745	0.007	0.301
8	(8 × 1)	923.830	7.809	0.473	0.009	0.303
12	(1 × 12)	603.962	11.945	0.459	0.005	0.310
48	(8 × 6)	151.574	47.596	0.458	0.008	0.303
96	(8 × 12)	76.576	94.211	0.455	0.009	0.310

From 2 hours
To 1min.17sec.

Compare XcalableMP with MPI

Parallelization	Execution Time (sec.)	Modified/Inserted Lines of Code
XcalableMP	1,840.942	32
MPI	1,817.042	53

3D Image (NZ,NX,NY)=(192,192,192)

96 threads execution

Higher productivity by XcalableMP than MPI w/o sacrificing performance

In general...

	Productivity	Performance
XcalableMP(High Level)	○	△
MPI(Low Level)	×	○

Conclusion

Hybrid parallelization of 3D atomic image reconstruction from X-ray fluorescence holograms with XcalableMP and OpenMP

- PC Cluster (8nodes, 96cores in total)
  - Grid size of 3D Atomic Image (8,192,192)
    - 94x speedup by 96 threads
  - Grid size of 3D Atomic Image (192,192,192)
    - 30 min. (1,841 sec.) with 96 threads
    - Estimated 2days with single core
- Inter-node parallelization with XcalableMP
- Intra-node parallelization with OpenMP
- High productivity and performance by XcalableMP

Future work

- Execution of 3D Atomic Image Reconstruction on supercomputers such as GPU cluster (Ito) at Kyushu University