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New Parallelization Model of Sequential Monte Carlo Analysis with Prediction-Correction Computing

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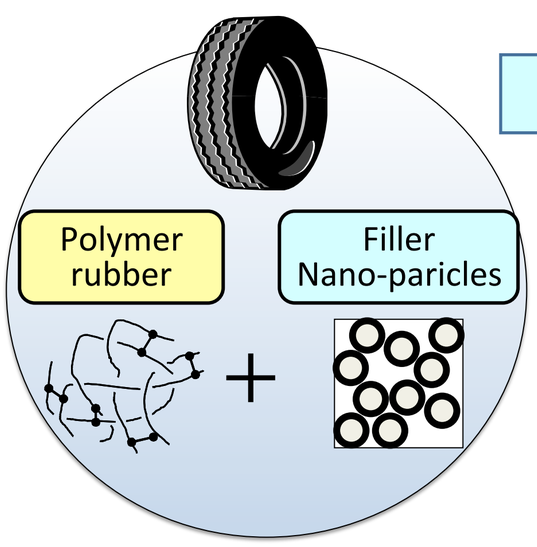
Inverse solving by sequential Monte Carlo analysis

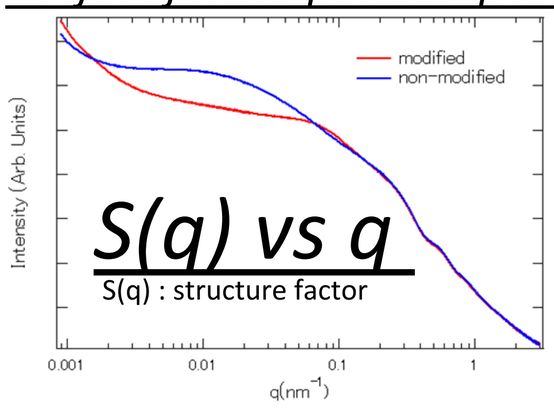
Building 3d model (particle positions) from X-ray scattering data.



SPring-8 @ JAPAN

courtesy of RIKEN/JASRI

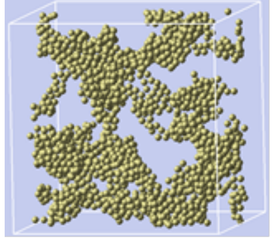
X-ray scattering data (S(q))
= info. of nano-partiles' positions

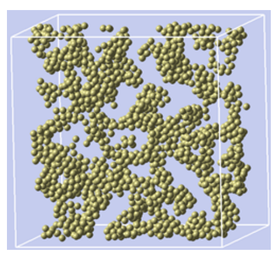


MC Search

$$g(r) = \frac{h(r)}{4\pi r^2 \rho}$$

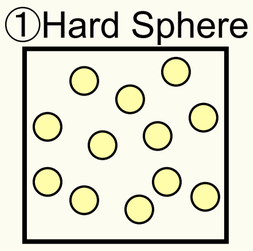
$$S(q) = 4\pi\rho \int_0^\infty dr r^2 (g(r) - 1) \frac{\sin(qr)}{qr} + 1$$



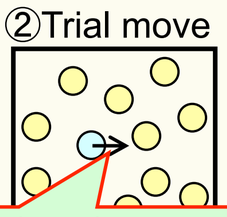


Algorithm of Conventional Reverse Monte Carlo method

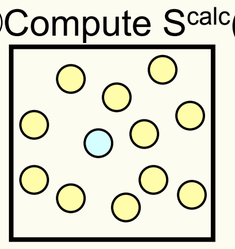
①Hard Sphere



②Trial move



③Compute $S^{calc}(q)$



④Compute error sum of square$\Delta\chi^2$

$$\chi^2 = \frac{\sum_q \left(S^{exp}(q) - S^{calc}(q)\right)^2}{\sigma^2}$$

Repeating it, χ^2 can be minimized.

→ Best estimated positions

$\Delta\chi^2 < 0$ → Accept

$\Delta\chi^2 > 0$ → Accept with the probability $\exp(-\Delta\chi^2/2)$

① Give initial configuration

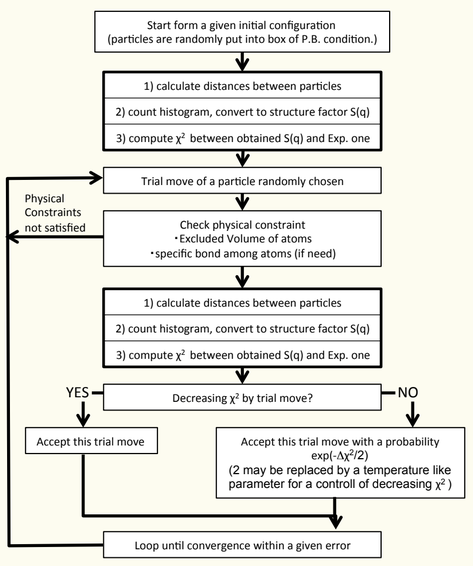
② Calculate S(q) and the change of χ^2 by trial move chosen satisfying with physical constrains

- χ^2 is a square sum of differences between S(q) obtained from configuration and Experimental data.

$$\Delta\chi^2 = \sum_q \frac{-2\left(S^{exp}(q) - S^{prev}(q)\right)\Delta S(q) + \left(\Delta S(q)\right)^2}{\sigma(q)^2}$$

③ Accept with the probability exp(-$\Delta\chi^2/2$)

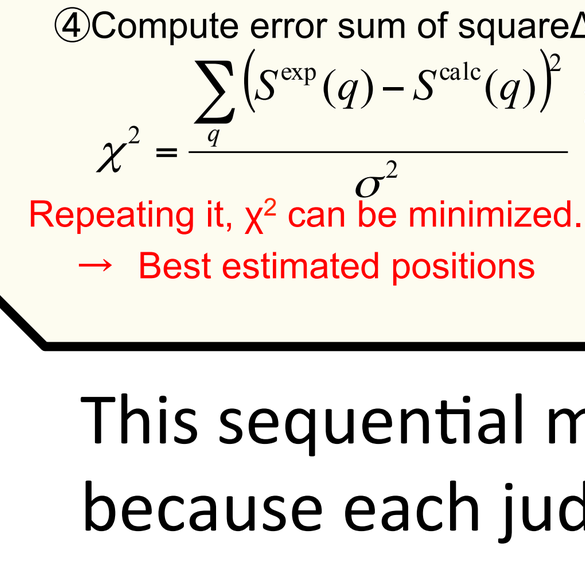
④ Until convergence

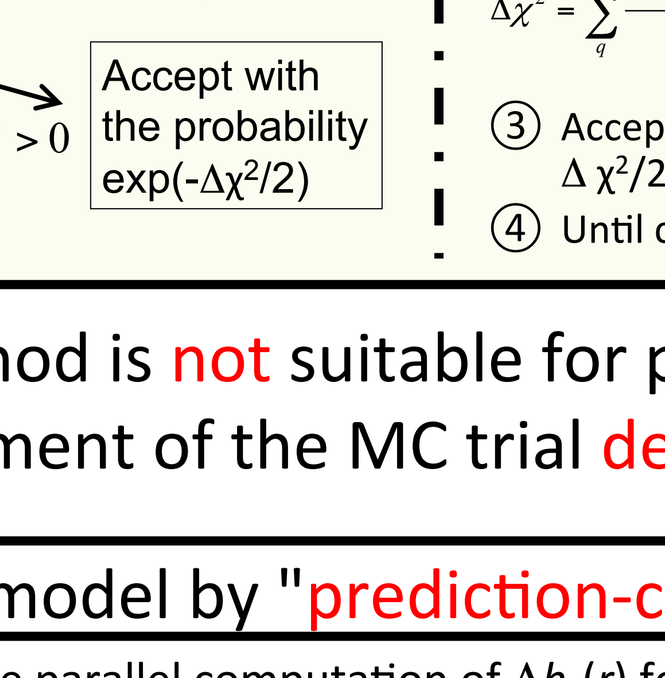


This sequential method is not suitable for parallelization because each judgement of the MC trial depends on its previous state.

New Parallelization model by "prediction-correction" method

Algorithm is changed to separate parallel computation of $\Delta h_k(r)$ for k = 1 to M and unparalleled correction part.
Communication overhead can be reduced to 1/M of that of "sequential" method.





"prediction" part calculates $\Delta h_k(r)$ M times simultaneously, where each $\Delta h_k(r)$ consists of an independent partcle move.

$\Delta h_1(r)$
$\Delta h_2(r)$ except for i_1-i_2
$\Delta h_3(r)$ ※i_1-i_2, i_1-i_3, i_2-i_3

Here, i_k is particle id of sampled as k-th trial.

"correction" part fixes $\Delta h_k(r)$, which were tentatively calculated for pairs of M trial particles in the prediction part.

$\Delta h_2(r)$ for i_1-i_2
$\Delta h_3(r)$ for i_1-i_2, i_1-i_3, i_2-i_3

For the efficiency, tentative $\Delta h_2(r)$ for i_1-i_2 is calculated in the prediction part. The tentative value is subtracted in the correction part.

Acknowledgement

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Performance analysis and optimization

Optimization for the histogram calculation kernel

```
do i=1+nid,n,nproc
  xtmp(:)=pos(:,i) + 3.0d0
!***     Loop1    ***
  do j=1,i-1
    dx(:)=(xtmp(:) - pos(:,j))*0.5d0
    dx(:)=2.0d0*(dx(:) - aint(dx(:)))-1.0d0
    r=ma*dx(1)*dx(1)+mb*dx(2)*dx(2)+ mc*dx(3)*dx(3)
     ilist(j)=sqrt(r)*drinv + 0.5d0
   enddo
!*** End of Loop1  ***
!***     Loop2   ***
  do ip=1,nthr
       ip_st = int((i-1)*dble(ip-1)/dble(nthr)) + 1
       ip_en = int((i-1)*dble(ip)/dble(nthr))
     do j=ip_st,ip_en
        phist(ilist(j),ip)=phist(ilist(j),ip) + 1.d0
      enddo
   enddo
!*** End of Loop2 ***
enddo

do ip=1,nthr
  do ir=1,nr
    mpihist(ir)=mpihist(ir)+phist(ir,ip)
  enddo
enddo
```

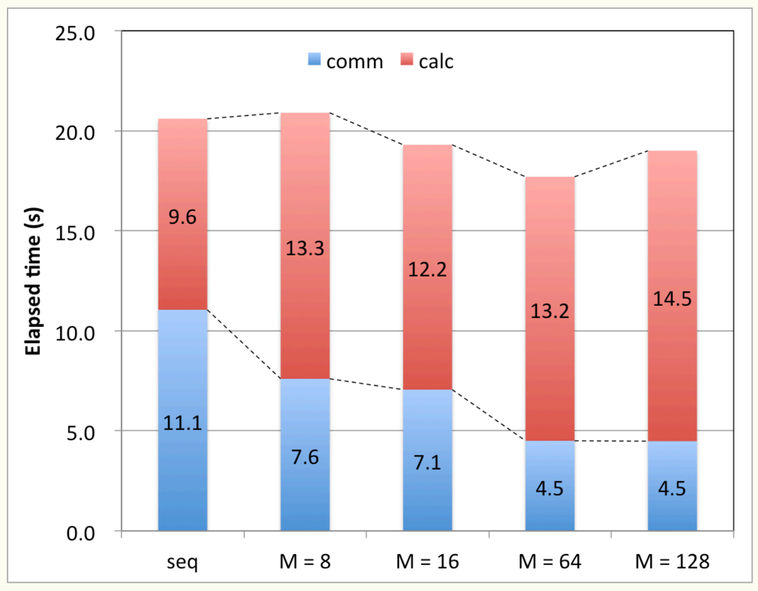
- We modified the original kernel loop for the single instruction multiple data (SIMD) hardware with fused multiply-add (FMA) support in terms of instruction-level parallelization.
- To prevent indirect memory access, we divided the kernel loop into two loops.
  (Loop1) distance computation for all particle pairs
  (Loop2) histogram reduction on each thread
- For Loop1, we achieved 51 % of theoretical peak.
- Total performance in both loops was 36.5 % where 75 % of the instructions were SIMD vectorized.

Estimation of Theoretical Limit of the Performance of Loop1.
Demand for memory: 16 bytes / Loop
Flop/Loop = 29 (including sqrt and aint functions.)
Byte/Flop = 0.55
Due to Limit (B/F=0.36) of K computer, 65 % is theoretical limit of Loop1.
Check of this limit with computation removing sqrt and aint.
Peak-ratio = 44.2 %. Flop/Loop = 26.01.
Validity of the estimated theoretical Limit is confirmed.

Performance of the "prediction-correction" computing

- comm time is reduced from 11.1 s to 4.5 s. It includes MPI_allreduce and MPI_bcast.
- In "prediction-correction" method, number of part of the MPI calls is reduced to 1/*M*.

- In 4,194,304-particle system, 24 nodes and *M* = 64 is sweet spot.The calculation time of $\Delta h(r)$ for *M* = 64 was 2.9 s (14 %) shorter than that of the "sequential" method.
- Our “prediction–correction” method is very useful for large-particle systems as well as large parallel computers.



Elapsed time of the $\Delta h(r)$ calculation on 24 nodes

Sequential	M=8	M=16	M=64	M=128
20.6 s	20.9 s	19.3 s	17.7 s	19.0 s

count of collective communication

MPI functions	Sequential	M=64
Allreduce	39,927	13,921
Bcast	153,236	14,337

We also benchmarked a 33,554,432-particle system on 256 nodes of the K computer; the elapsed time with *M* = 32 was 22.4 s, which is faster than that of the *M* = 64 run (24.7 s).

- For speed up of RMC computations, physical conditions such as excluded volume (EV) are checked before the $\Delta h(r)$ calculation.
- In this case, approximately 13 % of the 100,000 trails satisfied the EV conditions. Next, approximately 60% of the satisfied trials were accepted in terms of the χ^2 judgments.

- We achieved **36.5%** of peak performance on **“K computer”「京」** for the histogram calculation kernel.
  - 5.98 Tflops was achieved on 128 nodes with 4,194,304 particles.
  - 339 Tflops was achieved on 8,192 nodes with 33,554,432 particles.
- New algorithm "prediction-correction" is efficient.
  - The achieved speed up was 14% of the elapsed time.
  - Reduction of the MPI communications leads to reducing the elapsed time.