Problems in a large-scale calculation of atomic nuclei

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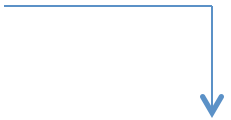
What we do:

Input information of nuclei
[functional of density expressing energy]

Dynamical equation
[matrix eigen equation (QRPA)]

Observables [energy, transition probabilities …]



Application:
How nuclei were created in the universe?

Computational problem

How to handle large data efficiently

^{172}Yb

5,000 wave functions of nucleons $F(r,z,\sigma=1,2)$

$F \leftarrow$ array of dimension 3000

0.12 Gb

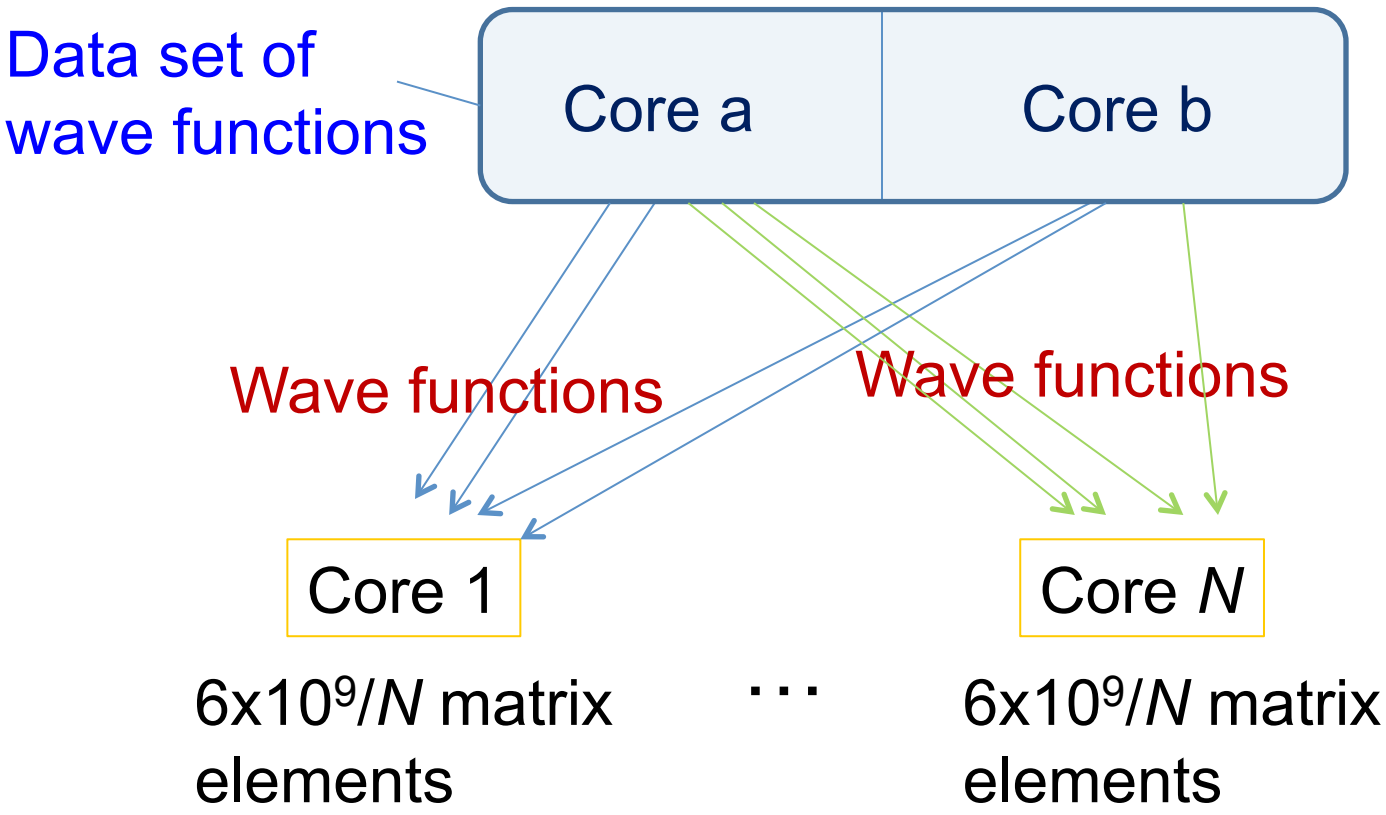
More is necessary in the future. Then, what can we do?

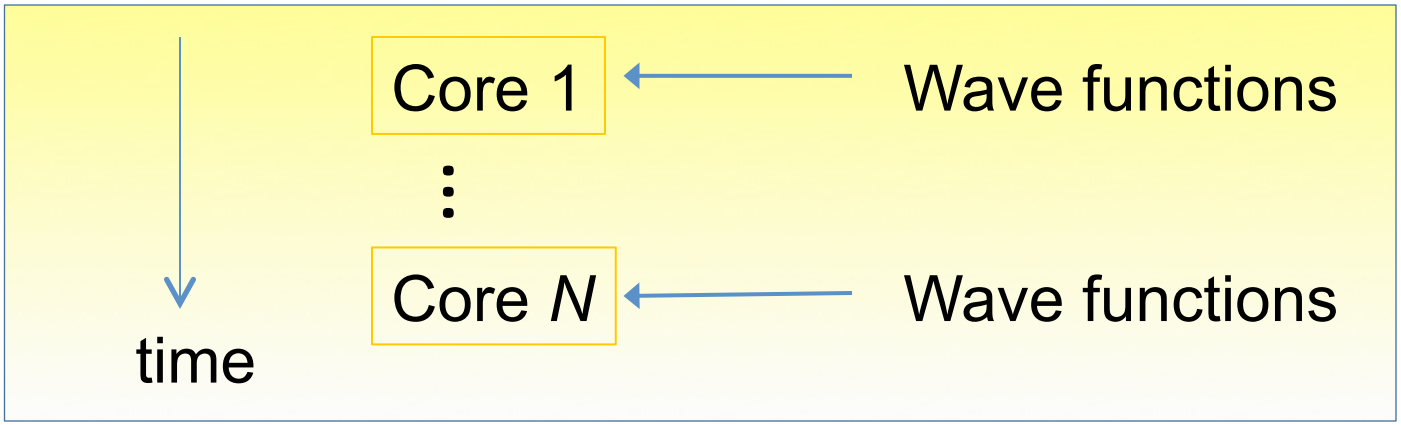
4 wave function

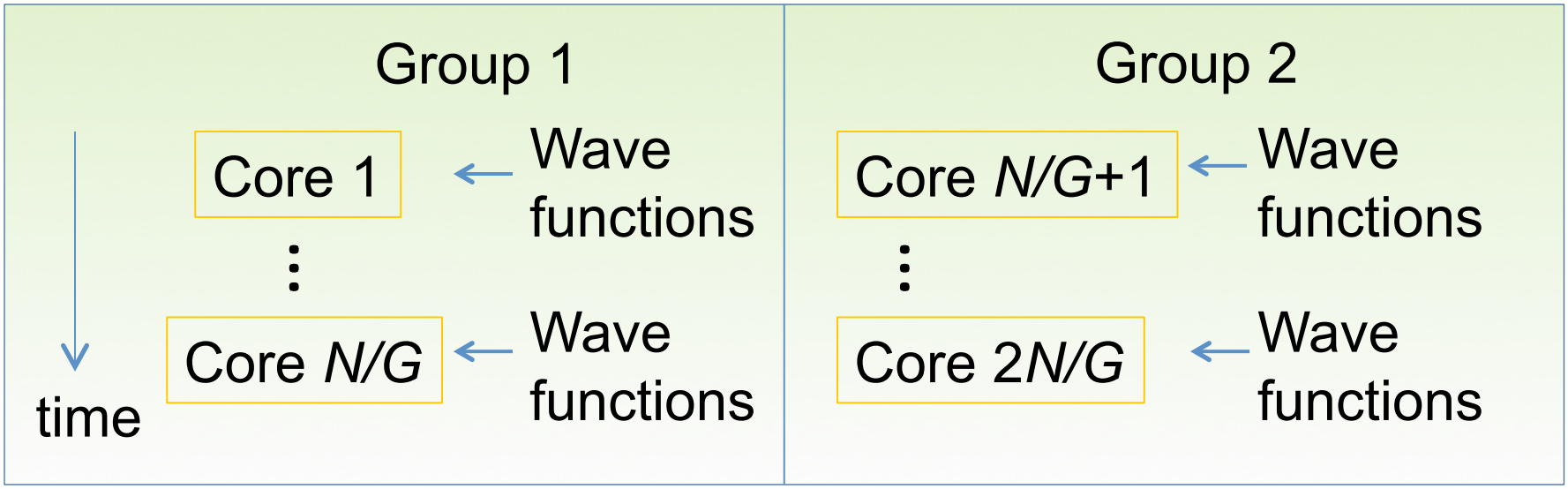
↓

A matrix element

6×10^9 matrix elements necessary to calculate


Data set of
wave functions
Core a
Core b
Wave functions
Wave functions
Core 1
Core N
6x10^9/N matrix elements
...
6x10^9/N matrix elements





The second scheme did not reduce the communication time.

We store 6×10^9 matrix elements in files.
What is efficient and safe I/O ?

Direct-access unformatted files are used

Sometimes writing error occurs, when multiple cores write data in different address.
The more cores used, the more often this problem occurs.