Importance of Selecting Data Layouts in the Tsunami Simulation Code

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Backgrounds

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HPC applications

- Playing important roles in various fields
- Tending to require high data transfer capability
  - E.g. Simulation applications
  - Demands for dealing with much data for calculations

Memory-intensive applications

- A sustained performance is limited by the memory performance of computing systems
  - The wide performance gap between processor and memory
- One of the challenge to accelerate memory-intensive applications is full exploitation of the memory performance
- A tsunami simulation as the target application in this research
  - A part of the real-time tsunami inundation forecast system

The real-time tsunami inundation forecast system

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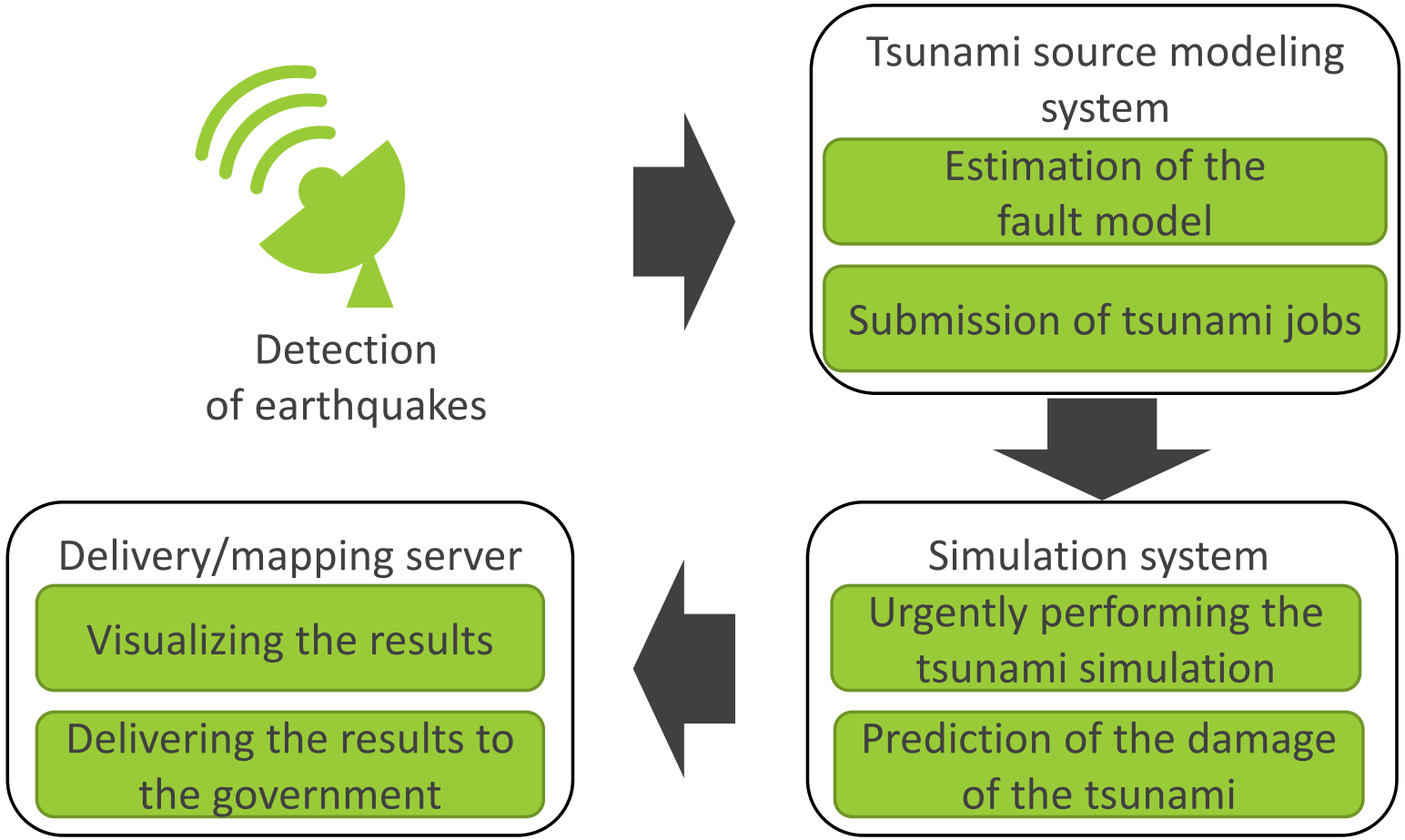
Overviews

- The system that helps to decide the appropriate actions for tsunamis' damage



The tsunami simulation

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Overviews

- Computational model :TUNAMI Model
  - Governing equations :Nonlinear shallow water equations
  - Numerical scheme :The staggered leap-flog finite difference method
- Outputs
  - The maximum inundation depth, the tsunami arrival time, the water level changes over time, and so on

Challenges

- Acceleration
  - Simulation of the damage in real time
- Achievement of high performance independent of target areas
  - The execution time varies depending on input data
  - It is impossible to predict the target areas where tsunami reaches

Objective & Approach

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Objective

- Acceleration of the tsunami simulation with various input data and computing systems
- Clarification of the necessity of the tuning strategy for selecting data structure depending on input data and computing systems

Approach

- Adapting typical types of memory-access-efficient data structures to the tsunami simulation
  - Discrete array
  - Array of structures
  - Structure of arrays
- Analyzing the performance variations

Data structures in simulation applications

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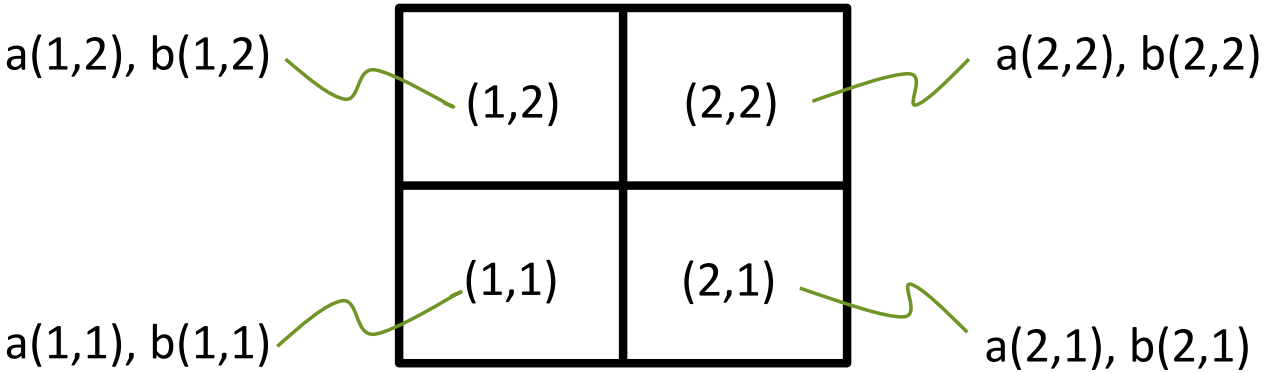
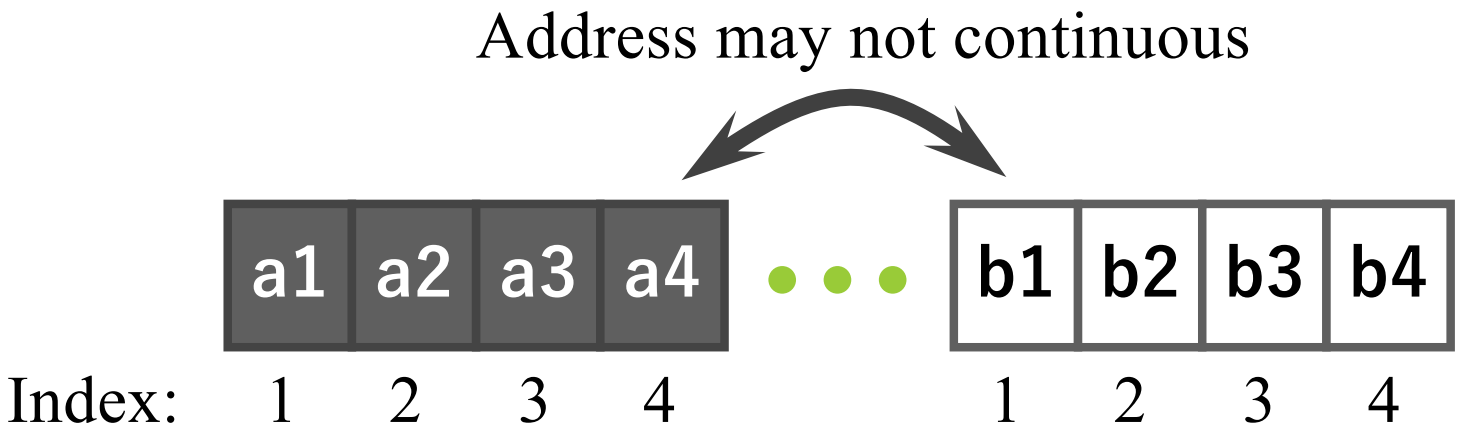
- Data definition in the numerical study of dynamics
  - Multiple physical values are defined for each point of a computation grid



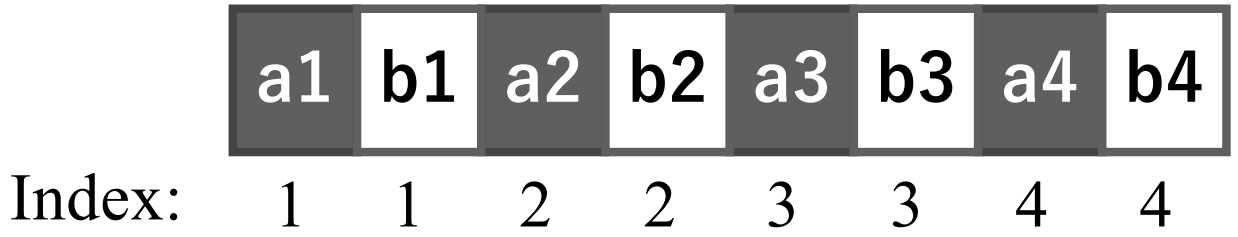
- Typical data structures where physical values are defined
  - Three types of typical data structures
    - Discrete arrays
    - Array of structures
    - Structure of arrays

Discrete arrays (**DA**)



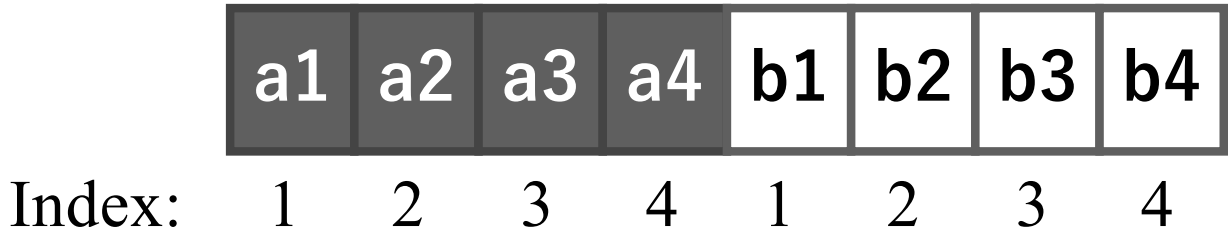
- Data layout on a memory
  - Physical values are stored in each array
  - Elements of physical values are stored in the order of index on a grid
    - ✓ Efficient memory accesses
  - Head addresses of arrays may be separated each other
    - × Inefficient memory accesses when accessing some arrays at once

Array of structures (**AoS**)



- Data layout on a memory
  - Data sets compose an array
  - Physical values of each grid are continuously aligned
    - ✓ Convenient to deal with physical values data of individual grid points
  - An element of a physical value is distant from another element
    - × Memory accesses may become inefficient

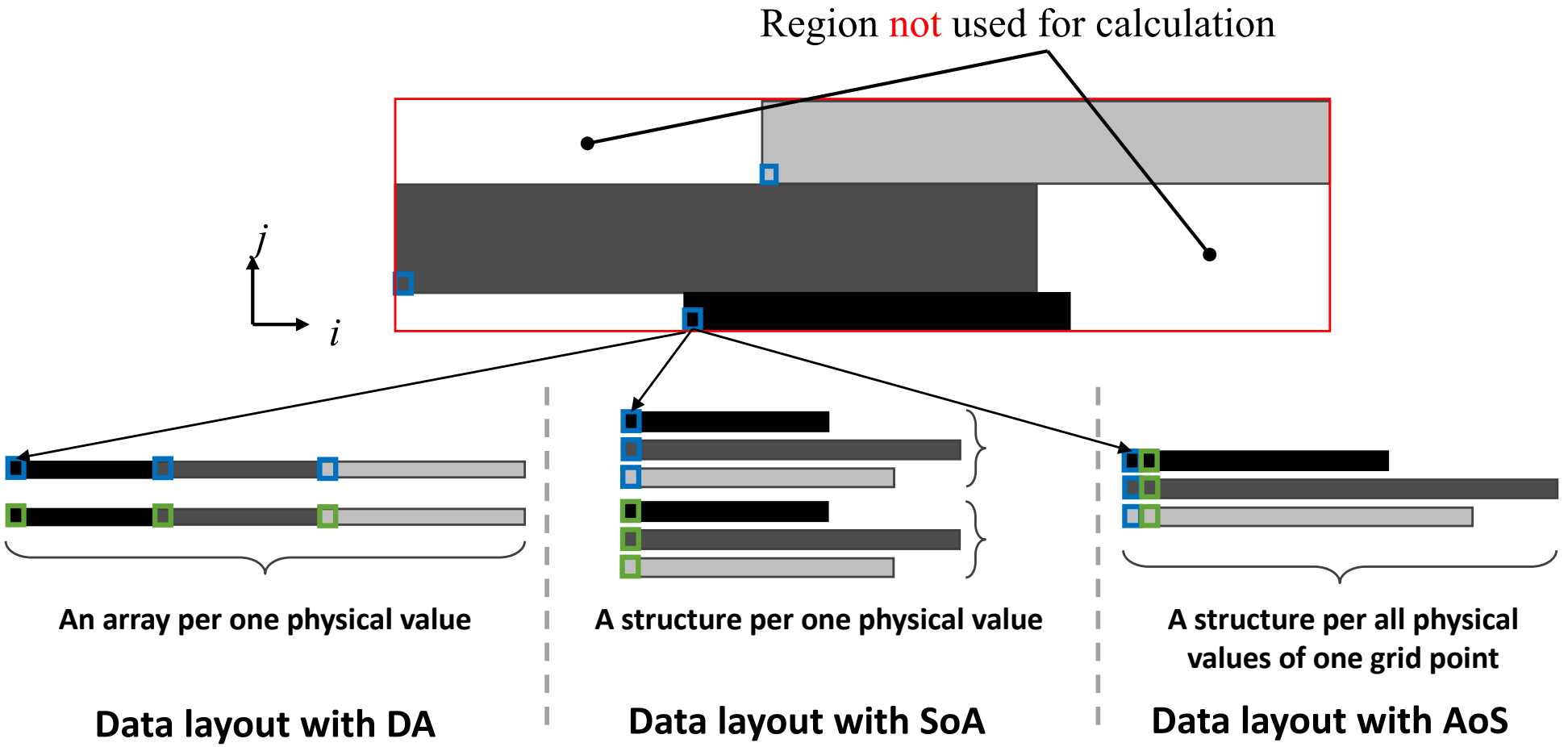
Structure of Arrays (**SoA**)



- Data layout on a memory
  - One data structure contains several arrays holding physical values
    - One array is provided for each physical value (same as the **DA** data layout)
  - Elements of the same physical values are placed closer on a memory
    - ✓ Efficient memory accesses
  - The arrays are also continuously aligned on a memory
    - ✓ Memory access may become more efficient than the **DA** data layout

Implementation of the tsunami simulation

- Concepts of three data layouts in the tsunami simulation



Implementation of the tsunami simulation

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Example codes

Code 4. The implementation of the *DA* data layout

```
 1:SUBROUTINE NLMNT2_DA
 2:···
 3:REAL,DIMENSION(BDLNG(N),2) :: ZL,ML,NL
 4:···
 5:DO K=1,NUMBLOCK(N)
 6:!$OMP DO PRIVATE(L,J)
 7:  DO J=1,JLNG(K,N)
 8:!$OMP SIMD
 9:    DO L=LJSTA(J,K,N),LJEND(J,K,N)
10:      ···
11:      XNNL=0.25*(NL(L,1)+NL(L+1,1)+NL(L-BIL,1)&
12:         +NL(L+1-BIL,1))
13:      FFXL=FN*SQRT(ML(L,1)*ML(L,1)+XNNL*XNNL)&
14:         /DDXL**(7.0/3.0)
15:      XML =(1.0-FFXL)*ML(L,1)&
16:         -GG*RX*DDXL*(ZL(L+1,2)-ZL(L,2))
17:      ···
18:    END DO
19:  END DO
20:END DO
21:···
22:END SUBROUTINE NLMNT2_DA
```

Code 5. The implementation of the *SoA* data layout

```
 1:SUBROUTINE NLMNT2_SOA
 2:···
 3:TYPE ZLST
 4:  REAL,DIMENSION(:) :: ZLS
 5:END TYPE
 6:TYPE MLST
 7:  REAL,DIMENSION(:) :: MLS
 8:END TYPE
 9:TYPE NLST
10:  REAL,DIMENSION(:) :: NLS
11:END TYPE
12:TYPE ALLD
13:  TYPE(ZLST),DIMENSION(:,:) :: ZL
14:  TYPE(MLST),DIMENSION(:,:) :: ML
15:  TYPE(NLST),DIMENSION(:,:) :: NL
16:END TYPE
17:TYPE(ALLD) :: ALLV
18:···
19:DO K=1,NUMBLOCKS
20:!$OMP DO PRIVATE(L,J)
21:  DO J=1,JLNG(K)
22:!$OMP SIMD
23:    DO L=LJSTA(J,K),LJEND(J,K)
24:      ···
25:      XNNL=0.25*(ALLV%NL(K,1)%NLS(L) &
26:         +ALLV%NL(K,1)%NLS(L+1) &
27:         +ALLV%NL(K,1)%NLS(L-BIL) &
28:         +ALLV%NL(K,1)%NLS(L+1-BIL))
29:      FFXL=FN*SQRT(ALLV%ML(K,1)%MLS(L) &
30:         *ALLV%ML(K,1)%MLS(L) &
31:         +XNNL*XNNL)/DDXL**(7.0/3.0)
32:      XML =(1.0-FFXL)*ALLV%ML(K,1)%MLS(L) &
33:         -GG*RX*DDXL*(ALLV%ZL(K,1)%ZL(L+1) &
34:         -ALLV%ZL(K,2)%ZL(L))
35:      ···
36:    END DO
37:  END DO
38:END DO
39:···
40:END SUBROUTINE NLMNT2_SOA
```

Code 6. The implementation of the *AoS* data layout

```
 1:SUBROUTINE NLMNT2_AOS
 2:···
 3:TYPE ELEMENTS
 4:  REAL,DIMENSION(:) :: ZL
 5:  REAL,DIMENSION(:) :: ML
 6:  REAL,DIMENSION(:) :: NL
 7:END TYPE
 8:TYPE BLOCKS
 9:  TYPE(ELEMENTS),DIMENSION(:) :: EMLS
10:END TYPE
11:TYPE(BLOCKS),DIMENSION(NUMBLOCKS) :: BLKS
12:···
13:DO K=1,NUMBLOCKS
14:!$OMP DO PRIVATE(L,J)
15:  DO J=1,JLNG(K)
16:!$OMP SIMD
17:    DO L=LJSTA(J,K),LJEND(J,K)
18:      ···
19:      XNNL=0.25*(BLKS(K)%ELMS(L)%NL(1) &
20:         +BLKS(K)%ELMS(L+1)%NL(1) &
21:         +BLKS(K)%ELMS(L-BIL)%NL(1) &
22:         +BLKS(K)%ELMS(L+1-BIL)%NL(1))
23:      FFXL=FN*SQRT(BLKS(K)%ELM(L)S%ML(1) &
24:         *BLKS(K)%ELMS(L)%ML(1) &
25:         +XNNL*XNNL)/DDXL**(7.0/3.0)
26:      XML =(1.0-FFXL)*BLKS(K)%ELMS(L)%ML(1) &
27:         -GG*RX*DDXL*(BLKS(K)%ELMS(L+1)%ZL(2) &
28:         -BLKS(K)%ELMS(L)%ZL(2))
29:      ···
30:    END DO
31:  END DO
32:END DO
33:···
34:END SUBROUTINE NLMNT2_AOS
```

Experimental environments

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Computing systems

Processor	Intel Xeon Gold 6126	Vector Engine Type 10B
Performance	1996.8 Gflop/s (SP)	4.30 Tflop/s (SP)
Memory subsystems	DDR4-2666	HBM2
Memory bandwidth	128 GB/s	1.22 TB/s
Memory capacity	192 GB	48 GB

Software environments

Compiler	Intel Compiler 19.0.5.281	NEC Compiler for VE 2.5.1
Options	-O3 -mcmodel=large -xCORE-AVX512 -qopt-zmm-usage=high -qopemmp	-O3 -fopenmp

Experimental environments

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Kernel code

- Extracted high-cost subroutine

Input data

- 12 computational domains that have possibilities to be suffered from significant damage of tsunamis
  - Computational domain composed of five-level resolutions: D1
  - Computational domains composed of four-level resolutions: D2~D12

Domain	Grid size (m)	D1	D2	D3	D4	D5	D6	D7	D8	D9	D10	D11	D12
		Number of grids											
1	810	1566720	2012940	2118960	2162160	2146320	2146320	2146320	2012940	2012940	2118600	2118600	2118600
2	270	1663200	1703484	1395072	551448	556416	944748	1421856	2098980	1703484	2149200	1246716	1246716
3	90	2887920	1807560	2284092	1524456	1315260	2023920	2704248	2475180	1807560	3178800	1409760	1301544
4	30	5969016	4983372	6295104	5405220	6525900	5757768	4133700	3424248	4983372	1990728	4539600	2907468
5	10	22795020	-	-	-	-	-	-	-	-	-	-	-

Evaluation results

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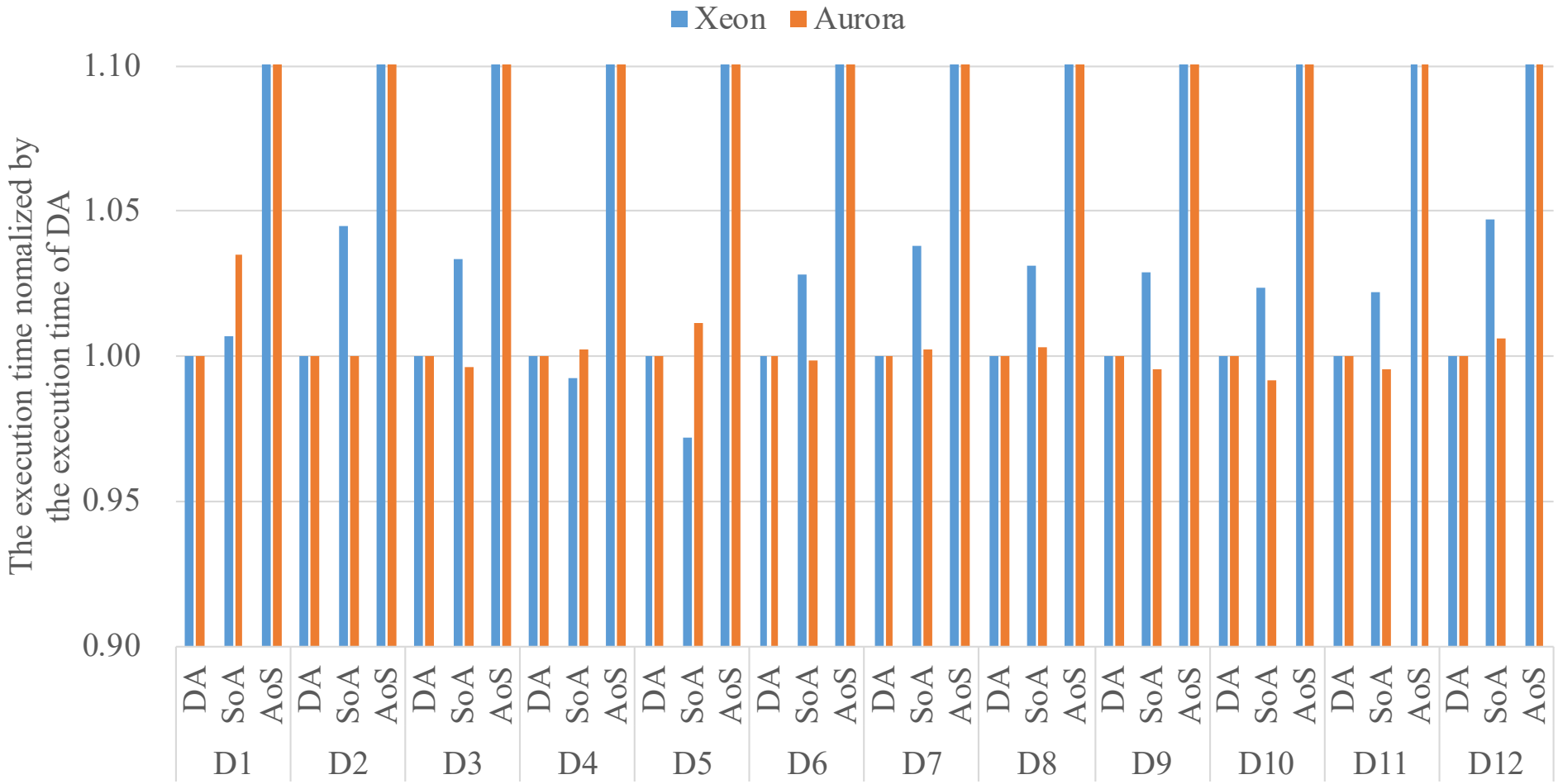
Execution times



Summary of the evaluation result

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Performances

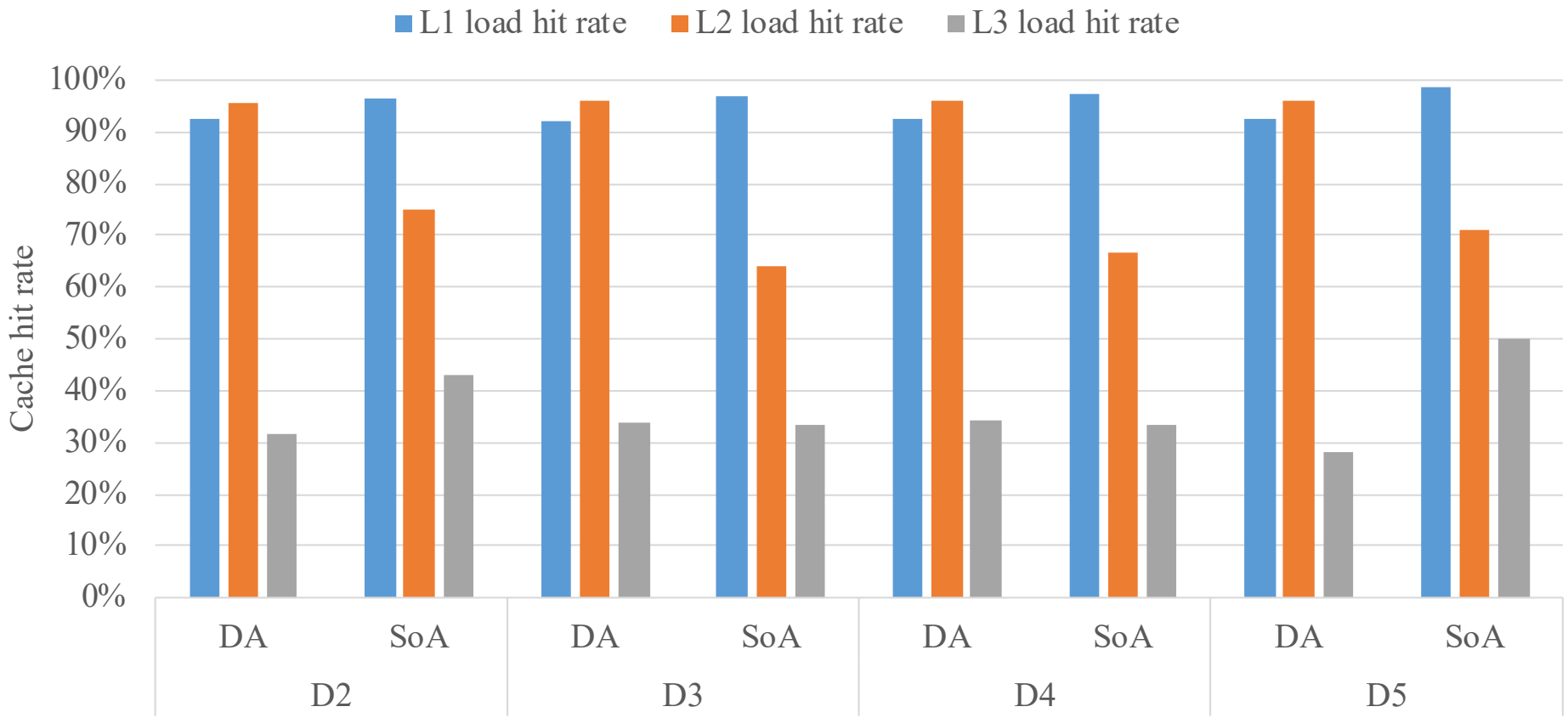
- DA and SoA achieves high performance
- AoS is always lowest performance
  - The overhead of accesses to scatteredly placed data elements
  - The requirement of much clock cycles for vector gather instructions

The variation of the performance

- The performance of the tsunami simulation is changed by
  - Computing systems
  - Data structure used in the code
  - Input data (target areas)
- Results indicates the necessity of appropriate selection of the data structure based on computing systems and input data

Detailed analysis

Cache load hit ratios on Xeon



Detailed analysis

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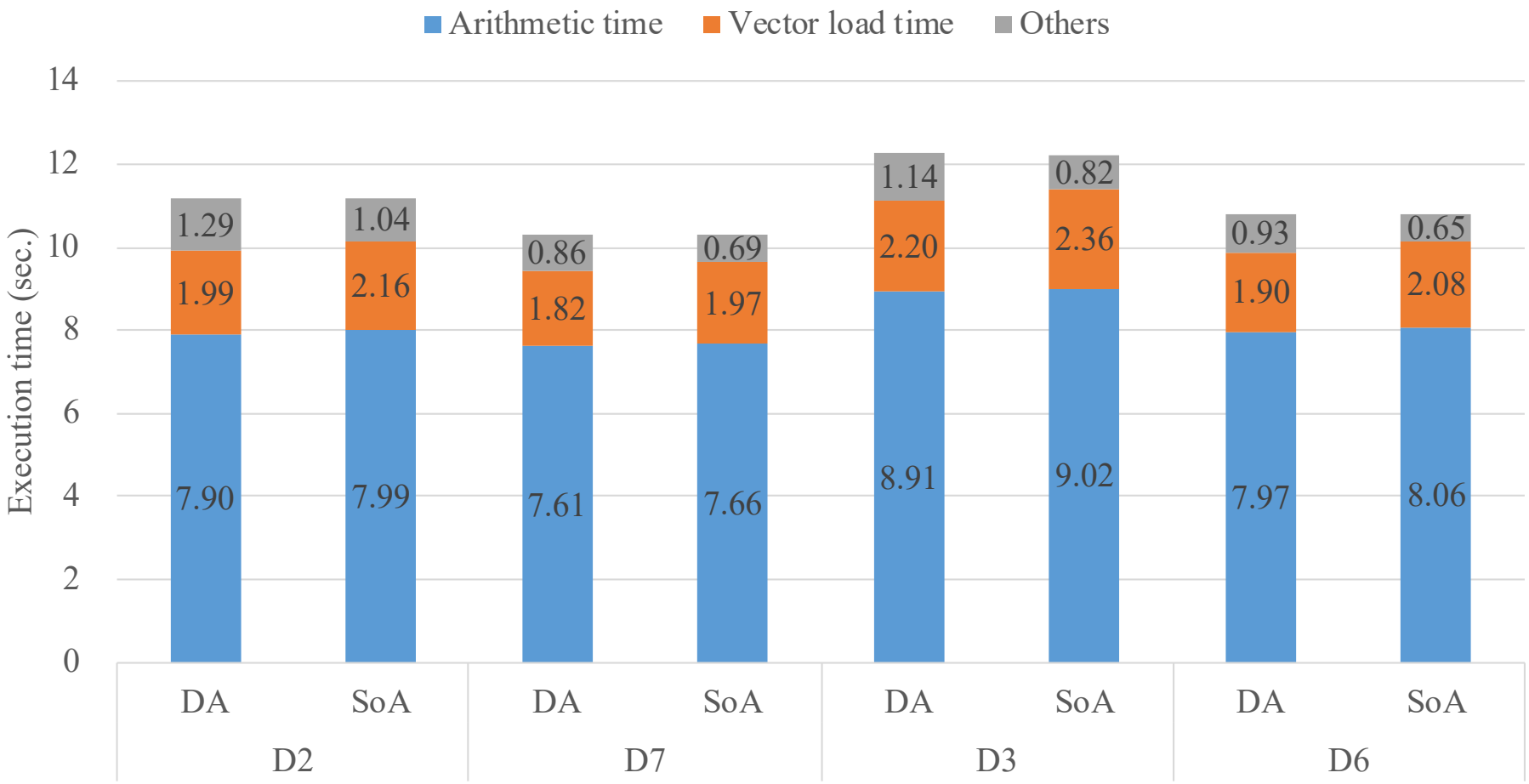
Breakdowns of the execution time on SX-Aurora TSUBASA



Summary of the detailed analysis

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Uncertainty of performance variation factor

- Xeon-based system
  - L1 cache load hit ratios are improved by using structure of arrays with all the inputs
  - L3 cache load hit ratios vary independent of data structure and inputs
- SX-Aurora TSUBASA
  - The arithmetic time and vector load time increase in DA and SoA with all the inputs
  - The execution time other than the arithmetic time and vector load time decreases with all the inputs

Necessity of more detailed analysis

- The complicated factors may affect the performance variation
- It is important to incorporate the selection of data structure into tuning techniques

Conclusions

- Tsunami simulation needs to be accelerated for real-time executions regardless of target areas

- This research focuses on selecting the data layout used in the tsunami simulation for efficient memory accesses
  - DA, AoS, and SoA

- From evaluation results,
  - Combinations of the computing systems, data layouts, and input data change the performance of the tsunami simulation
  - The factor of performance variation is unclear from the simple analysis
  - More detailed analysis is necessary for establishing a technique to tune the data layout

Future work

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- More detailed analysis
  - Factors affecting the performance variation
  - Clarification of the relationship among performance, input data, data layout, and computing systems
- Establishment of tuning technique
  - Selection of data layout based on;
    - Computing systems
    - Target applications
    - Input data

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