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Compression of Scientific Simulation Data by Stochastic Basis Expansion - Example on Multiple Computer Systems

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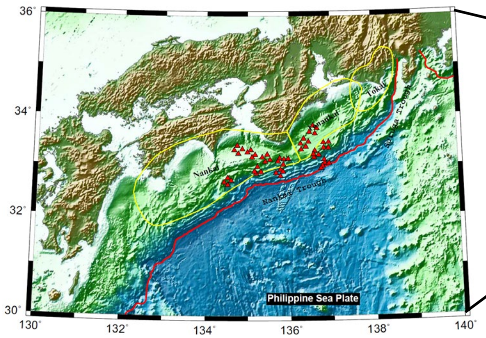
Introduction

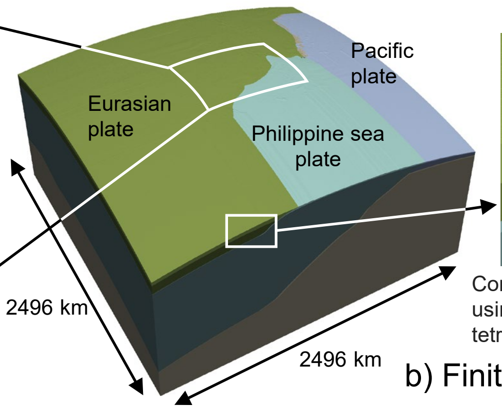
- High-performance parallel and distributed storage systems are being developed to enable scientific data storage and processing
  - Here, information about the structure and temporal evolution of phenomena is extracted by storing and processing data of the target phenomena
- For large-scale complex problems, the space in which the phenomenon takes place is especially large, and amount of data is enormous
  - Important to develop both high-performance data storage systems and algorithms that effectively utilize these systems for data compression, restoration, and analysis

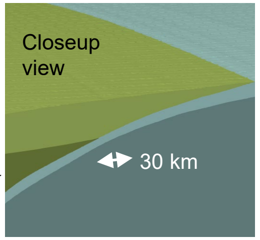
Example of large-scale complex problem

- Uncertainty quantification for earthquake simulation: important as crustal information is not known precisely
- Since the size of crustal deformation simulation is huge (1.3×10^{11} degrees of freedom), uncertainty quantification requiring 10000 cases of crustal deformation analysis cannot be conducted as data becomes $1.3 \times 10^{11} \times 10000 = 1.3 \times 10^{15}$ degrees of freedom
- We develop a method to generate compressed data of many cases of simulations by stochastic basis expansion to enable uncertainty quantification of such large-scale problems



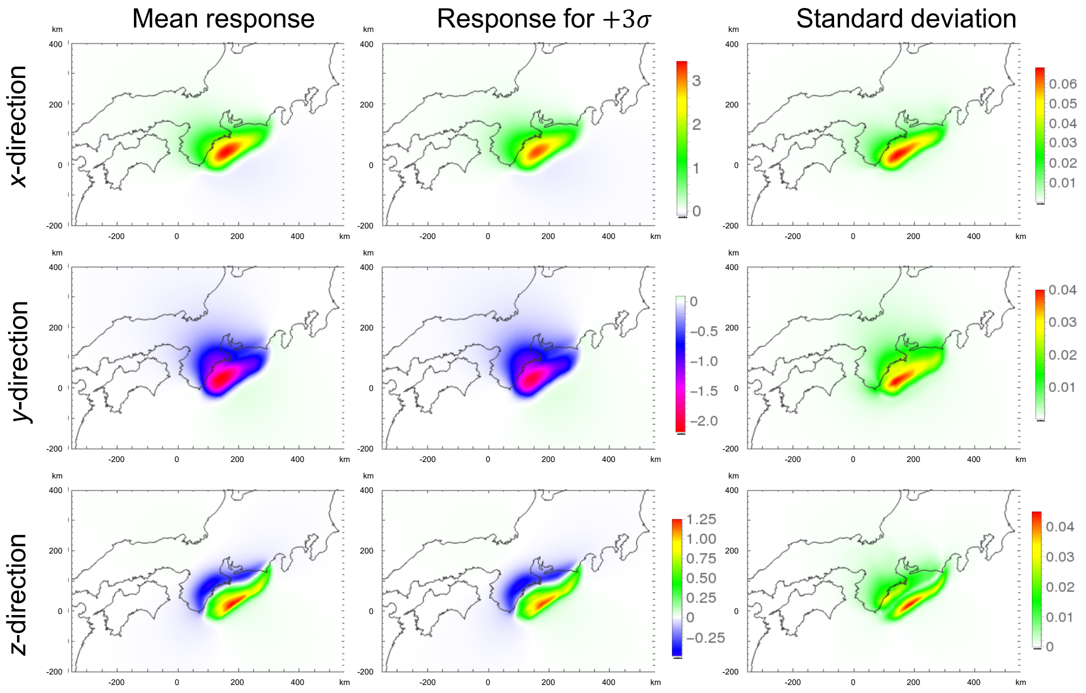
a) Target area



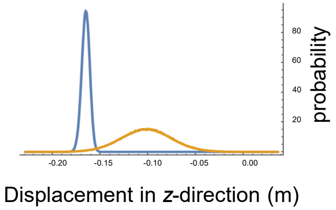


Complex geometry discretized using 375 m second-order tetrahedral elements

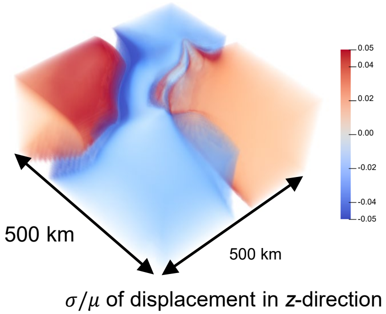
b) Finite-element model



c) Stochastic response at surface (displacement (m))



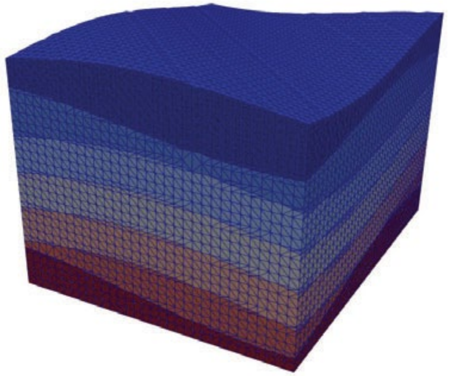
d) Stochastic response at two points on surface



e) Stochastic response shown in 3D

Reduction of Monte Carlo simulation data

- Expand results of many-case simulations using stochastic basis, and store only the coefficients for each basis
  - Response data expanded as $\boldsymbol{u} = \Sigma_{p=0}^{n_{PC}} \Psi_p \boldsymbol{u}^{(p)}$ in the stochastic space, where Ψ_p are the stochastic bases and $\boldsymbol{u}^{(p)}$ are components in physical space using finite-element discretization
- Example for crustal deformation problem:
  - Results obtained by running deterministic simulations (corresponding to a Monte Carlo simulation sample) and the response results reconstructed from the stochastic basis expansion match with high accuracy
  - Response results for many Monte Carlo simulations can be reconstructed accordingly



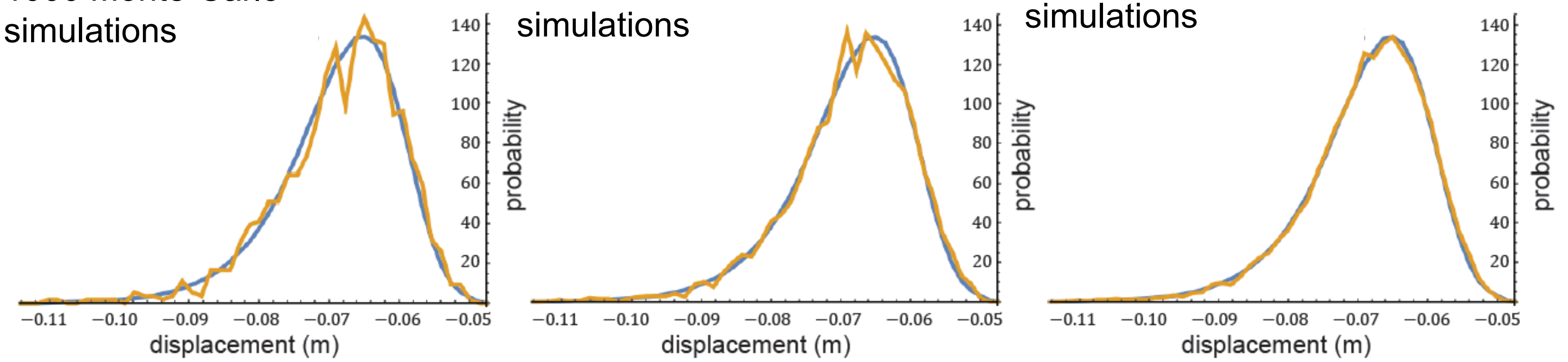
Problem with normal distribution in material properties

Compute displacement response to input fault slip

1000 Monte-Carlo simulations

5000 Monte-Carlo simulations

10000 Monte-Carlo simulations



Blue line: probability distribution obtained by the developed method

Results for 10000 Monte Carlo simulations can be reconstructed with small data size

Data size reduction rate and computation cost

- Data storage size can be reduced by 10000 / 286 = 35-fold by use of the proposed method:
  - 10000 cases of Monte Carlo simulations are typically required for considering the convergence of the response probability distribution
  - For a problem with 10 random variables, third-order stochastic basis expansion, which is considered sufficient for convergence of response, can be stored with the data size equivalent to 286 cases of deterministic simulations
- However, high-order stochastic expansion leads to large computation costs

Reduction of computation cost

- Based on the expansion calculations using stochastic bases conducted in the numerical analysis field, we developed a scalable algorithm that can efficiently utilize high-performance computer systems [1] for suppressing analysis costs involved in high-order expansions
  - Implemented on CPU-based Fugaku: up to 1.3×10^{11} degrees of freedom (DOF) x 10000 cases = 1.3×10^{15} DOF is reduced by 35-fold to 3.7×10^{13} DOF using nearly full Fugaku (147456 nodes)
  - Implemented on GPU-based Frontier: up to 3.7×10^{14} DOF data set is reduced by 35-fold using 5120 nodes of Frontier

[1] T. Ichimura, et al., “Extreme Scale Earthquake Simulation with Uncertainty Quantification,” SC22 Gordon Bell Prize Finalist, 2022.

Summary

- Developed a method that generates compressed large-scale simulation data by use of stochastic basis expansion
- Development of a scalable algorithm led to a 35-fold reduction in data size for problems up to 10^{15} degrees of freedom by use of CPU-based Fugaku and GPU-based Frontier
- With the developed method, we enabled uncertainty quantification of large-scale crustal deformation problem of 1.3×10^{11} degrees of freedom

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