Large-Scale Simulation of Groundwater Flow and Radioactive Nuclide Transportation

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In this study, we will optimize the simulation codes for radio nuclide transportation and groundwater flow on the Earth Simulator and conduct large-scale simulation for more than 106 years on the models of real disposal sites using these optimized codes. The results of the simulations will be helpful for making decision of final disposal sites. In this area of research we have various kinds of simulation codes. We will develop an infrastructure for large-scale simulations which consists of common and fundamental capabilities, such as parallel I/O for large-scale data sets, parallel visualization and parallel linear solvers. This infrastructure will be useful for optimization of developing codes and new codes on the Earth Simulator.

The VR code, a repository performance assessment code with multiple canister model, is ported and optimized to Earth Simulator in this year. The VR code was parallelized and vectorized so that vectorization ratio of 95.97%, and parallelization ratio of 99.35% are achieved. The demonstration calculation with one-thousand canister model is performed.

Keywords: High-level radioactive wastes, Performance assessment, Repository, Multiple canister model, Realistic model, Large-scale simulation

1. Introduction

A geologic repository for the high-level radioactive waste (HLW) where forty thousand canisters are to be disposed of is planned in Japan.

The HLW disposal business in Japan shifted from the research and development stage to the business stage by the establishment of Nuclear Waste Management Organization of Japan in 2000. The site selection of the repository is the next stage of the disposal business. It is assumed that the optimization of the repository design under the geological environment of the repository location, and the safety performance assessment of the repository considering repository layout will be performed after the repository site selection.

The conventional safety performance assessment of the Japanese HLW repository is summarized in H12 report [1]. As the purpose of the conventional Japanese performance assessment is to demonstrate the feasibility of the HLW repository in Japan, performance assessment is based on the conservative assumptions.

For example, the conventional performance assessment utilized the single-canister configuration model, under the assumption that all canisters are identical and interference effects between canisters on the radionuclide release and transport are negligible.

The performance assessment based on the realistic repository model is needed to perform the optimization of the repository design, and the repository performance assessment considering repository layout.

In recent years, the Virtual Repository (VR) code TM [1] for a multiple canister repository model has been developed by some of the authors [2][3][4]. The model utilized in the code includes the effect of multiple canister interaction by considering a one-dimensional compartment array in the direction of groundwater.

In the performance assessment of the HLW repository, the simulation time of more than one million years is needed to evaluate the repository performance. In the previous studies by some of the present authors, the VR code is executed using a PC cluster, so the total numbers of canisters in repository model is limited to a few hundred due to the limit of the computational ability of a PC.

In reality, however, the groundwater is assumed to meander through the repository, so the total numbers of canisters

[1] Virtual Repository code TM is the property of the University of California.

along the groundwater path is assumed to be more than one hundred.

In this project, the VR code was ported and partially optimized to ES. The purpose of the project is to execute the performance assessment of the HLW repository in practical time by using the full-scale repository model with forty thousand canisters by using the VR code.

2. The Main Characteristics of the Code

The primary characteristics of the VR code are as follows:

(1) Flexible module structure by applying object-oriented approach

The VR code has module structure and framework for multiple canister model by applying object-oriented approach. It is possible to reconfigure solvers flexibly without changing the other part of the code. The code is written by C++ language.

(2) Parallel calculation by using MPI

The VR code has the parallel calculation function by using MPI to solve the large calculation load of multiple canister repository model.

(3) Performance assessment by using multiple canister repository model

The VR code is able to simulate the effect of multiple canister interaction by considering a one-dimensional compartment array in the direction of groundwater. The planned HLW repository in Japan is shown in the Figure 1.

The repository is modeled as the array of compartments positioned in the direction of groundwater flow. The compartment is composed of glass, overpack, buffer, and Near-Field rock. (Figure 2)

Glass, overpack, buffer, and Near-Field are modeled as plates in the compartment model. The radionuclide released from the glass diffuses through the buffer to the Near-Field, then transported by groundwater to the neighboring compartment in the downstream side.

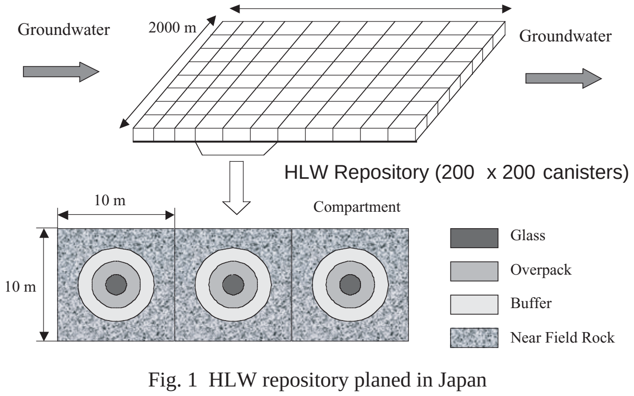

Fig. 1 HLW repository planed in Japan

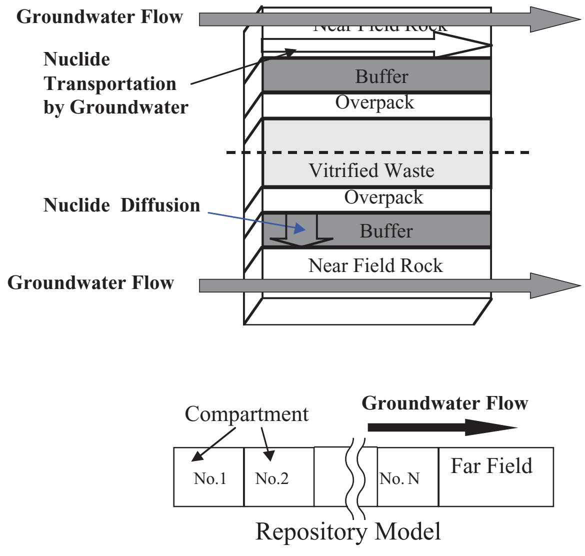

Fig. 2 Compartment Model

The calculation models utilized in the solvers of VR code are as follows:

– Glass model

Glass inventory is obtained by the solubility limit and congruent release model considering radionuclide decay. The governing equation is discretized by finite difference scheme.

– Buffer model

Buffer concentration is obtained by one-dimension non-steady state diffusion model considering radionuclide decay and retardation. The governing equation is discretized by finite difference scheme, and solved by implicit time integration scheme.

– Near-Field model

Near-Field concentration is obtained by non-steady state complete mixed tank model considering radionuclide decay and retardation. The governing equation is discretized by finite difference scheme, and solved by explicit time integration scheme.

– Far-Field model

Far-Field accumulation is obtained by non-steady state point model considering radionuclide decay. The governing equation is discretized by finite difference scheme.

3. The Code Optimization

The VR code was modified to be parallelized by Hybrid MPI/microtask method, in which node-wise calculations are parallelized by MPI, and intra node calculation is parallelized by microtask. The intra node calculation was modified to be vectorized.

The following program modifications are made to optimize the code in ES.

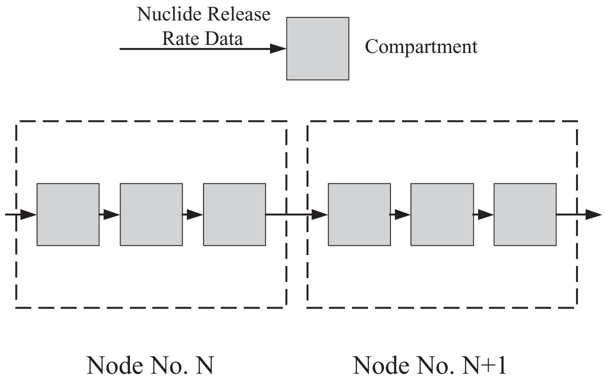

Fig. 3 Parallelization of node-wise calculation

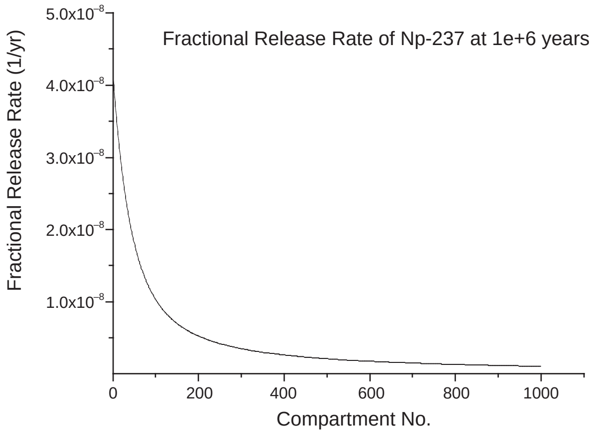

Fig. 4 Fractional Release Rate for various Canister Models

(1) Parallelization of node-wise calculation

The whole calculation is decomposed by assigning the same numbers of canister-wise calculations to each node. The nuclide release data between canisters in the most downstream and upstream side of the nodes are communicated by MPI. (Figure 3)

(2) Parallelization and vectorization of intra node calculation

One canister calculation contains glass, buffer, Near-Field calculations. The glass, and Near-Field calculations in the original code used in a PC cluster are executed in triple loop structure, which are composed of nuclide chain, nuclide member, and compartment number loops. The original buffer calculation is executed in fourfold loop structure, which are composed of nuclide chain, nuclide member, compartment, and mesh number loops.

Concerning the glass, and Near-Field calculations, the loop structure of the calculations is converted to the double loop structure, in which the outer loop is used to by microtask parallelization and the inner loop by vectorization.

The loop structure of the buffer calculation in a node is converted to the triple loop structure, in which the most outer loop is used by microtask parallelization, and the most inner loop is used by vectorization. The middle loop corresponds with mesh loop of tri-diagonal matrix inversion scheme, which cannot be parallelized nor vectorized.

4. Calculation Results

The code was optimized for parallelization and vectorization in H15, and vectorization ratio of 95.97% and parallelization ratio of 99.35% were achieved. The optimization of the code will continue in the next year.

The optimized code is used to execute performance assessment calculation with one-thousand canister model. The environmental impact of the repository is obtained by varying the total numbers of canisters from one to one thousand in the repository model. The nuclide release rate for Np-237 is used as the environmental impact index.

The nuclide decay chain composed of Cm-245, Am-241, and Np-237 is used in the input parameters. The simulation time of one million years, groundwater velocity of 1 m/yr, and Near-Field rock porosity of 0.5 are used as the input parameters.

The distribution of the Np-237 fractional release rate, the nuclide release rate from Near-Field to Far-Field divided by initial inventory including precursors, at the time of 1.0E+6 years is obtained and shown in the Figure 4.

The performance assessment with a few hundred canisters model is the largest simulation for conventional PC cluster calculation, but the simulation with over one thousand canisters is possible in Earth Simulator. It is shown from the Figure that as the canister number increases, the Np237 fractional release rate decreases due to the concentration interference effect.

The extension of available Earth Simulator nodes by code optimization for parallelization and vectorization in order to achieve repository performance assessment with forty-thousand canister model is the study theme in the next year.

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