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High-performance Supercomputing as a Risk Evaluation Tool for Geologic Carbon Dioxide Storage

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Abstract

Numerical modelling is a vital tool for predicting the behavior and fate of CO_2 in reservoirs as well as its impacts on subsurface environments. Recently, powerful numerical codes that are capable of solving coupled complex processes of physics and chemistry required for such modeling works have been developed. However they are often computationally demanding for solving the complex non-linear models in sufficient spatial and temporal resolutions. Geological heterogeneity and uncertainties further increase the challenges in modeling work, because they may necessitate stochastic modeling with multiple realizations. There is clearly a need for high-performance computing. In this study, we implemented TOUGH2-MP code (a parallel version of multi-phase flow simulator TOUGH2) on two different types (vector- and scalar-type) of world-class supercomputers with tens of thousands of processors in Japan. The parallelized code generally exhibited excellent performance and scalability after adequate tune-ups of the code. Using the code and the supercomputers, we have been performed several computationally demanding simulations. In this paper, we present the performances of parallel computation of the code measured on the two supercomputers. Then the following two examples are presented: 1) a highly heterogeneous high-resolution model, representing irregular nature of sand/shale distribution; 2) "Dissolution Diffusion Convection Process", which is expected to significantly enhance the dissolution trapping. Through the above two examples, it is illustrated that the spatial resolution of numerical model can critically change the evaluation of the effectiveness of CO_2 trapping mechanisms, demonstrating the necessity of supercomputing techniques for evaluating these risks more accurately.

Keywords: CO_2 storage; parallel computing; heterogeneity; interfacial instability; The Earth Simulator

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1. Introduction

Numerical modelling is a vital tool for predicting the behavior and fate of CO_2 in reservoirs as well as its potential impacts on subsurface environments. The numerical modeling involves multiphase flow of supercritical CO_2 and water with complicated processes such as diffusion and dispersion. Furthermore, in the risk assessment of geologic CO_2 storage, coupled flow simulations with geomechanics / geochemistry may be required for evaluating chemical and mechanical impacts of CO_2 injection on the integrity of the storage system (e.g., caprocks, and wells), and on subsurface environments (e.g., surface uplift due to fluid pressurization, and groundwater contamination). The modeling also involves heterogeneities in geologic media at many different length scales from wellbore- to basin-scale.

Recently powerful numerical codes that enable the above-mentioned capabilities have been developed, but they are often computationally demanding for solving problems in sufficient spatial and temporal resolutions. Geological heterogeneity and uncertainties are other aspects of the challenges in modeling work, because solving two-phase fluid flow problem in highly heterogeneous media is time-consuming, and moreover, for assessing geologic uncertainties, stochastic simulations with multiple realizations would be necessary. There is clearly a need for high-performance computing. Recently, massively parallel computation techniques using hundreds to thousands of processors have been developed and applied for geologic CO_2 storages [1][2].

In this study, we implemented TOUGH2-MP code [3], which is a parallel version of multi-phase flow simulator TOUGH2 [4][5] on two different types (vector- and scalar-type) of world-class supercomputers with tens of thousands of processors in Japan (i.e., The Earth Simulator2 and The T2K Open Supercomputer). This paper begins with descriptions of the implementation and modification of TOUGH2-MP code on these two supercomputers. This is followed by two illustrative example simulations, both are computationally demanding: 1) two-phase flow simulation for a highly heterogeneous, high-resolution model, representing irregular nature of sand/shale distribution in multi-million grid cells; 2) "Dissolution Diffusion Convection Process", which is expected to significantly enhance the dissolution trapping, but it requires very fine grids in mm to cm order to accurately simulate the process.

2. Code Implementation and modification

2.1 The Earth Simulator2 (vector-type supercomputer)

The Earth Simulator (ES) is a massively parallel vector supercomputer operated by JAMSTEC, originally developed for, and extremely used in, global climate change simulations. The ES had been the most powerful supercomputer in the world from 2002 to 2004, and recently it was upgraded to new ES2 in March 2009. ES2 is an NEC SX-9/E system and consists of 160 nodes with eight vector processors (the peak performance of each processor is 102.4Gflop/s) and 128 GB of computer memory at each node. For a total of 1280 processors and 20 TB of main memory, the total peak performance is 131 Tflop/s.

We have ported TOUGH2-MP to the Earth Simulator since 2008, but a special tune-up to increase its vector operation ratio (VOR) was needed for the efficient use of the ES vector processors. The original source code of TOUGH2-MP over 40,000 lines was originally written assuming the use on scalar computers. Thus it contains many obstacles for increasing the vector operation ratio, such as frequent conditional branches and short loop lengths. Especially deadly short loop lengths in the matrix solver were found to be the key issue of the improvement, because it limits upper bound of the average vector length and thus decreases the vector operation ratio that should be 95% or more to get reasonable performance on the vector architecture computer. In the original code, an iterative parallel linear solver package Aztec [6] was employed. The Aztec solver uses a distributed variable block row (DVBR) format (a generalization of the VBR format) as a matrix storage format, which is highly memory-efficient; however the innermost loop is relatively short, order of number of off-diagonal components for matrix-vector operations.

In order to achieve efficient parallel/vector computation for applications with unstructured grids, the following three issues are critical [7]: (1) local operation and no global dependency, (2) continuous memory access, and (3) sufficiently long innermost loops for vectorization. Nakajima [7] suggested that DJDS (descending-order jagged diagonal storage) reordering is suitable for efficient length of innermost loops, producing 1D arrays of coefficient with continuous memory access and sufficient length of innermost loops. Based on the considerations, we replaced the Aztec solver to a matrix solver in GeoFEM [8] that employs DJDS format and has been optimized for various massive parallel computers. In addition, we performed loop-unrolling and inline expansion wherever possible and effective, and rewrote bottleneck computations (loops) in the fluid property (EOS) module.

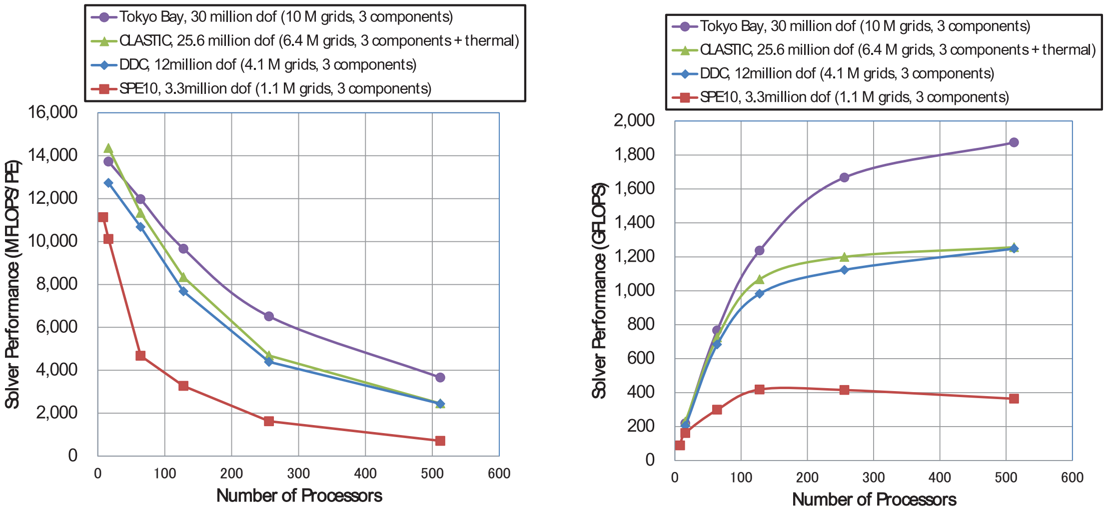
2.2 T2K Open Supercomputer System (scalar-type, massive cluster system)

The T2K Open Supercomputer System (Todai Combined Cluster) is a massive cluster system that consists of about 15,000 scalar-type processors and total memory 32TB with the total peak performance 140 Tflop/s, operated by The University of Tokyo. The T2K system consists of 952 nodes of Hitachi HA8000-tc/RS425 technical servers. Each node is built with the TYAN TN28 B4988 server, four Quad-Core AMD Opteron 8300 Processors (9.2GFlops), 128GB memory, and 1,000GB HD Bay. TOUGH2-MP has been running on T2K since 2010, but the optimization of the code on T2K is still underway.

2.3 Performance Measurements

On The Earth Simulator2, the modified code gained more than 60 times faster than the original code with Aztec solver. The effective speed of the new solver on ES2 is 10-14 GFlops/PE (10-14% of peak performance; VOR > 99.5%; Figure 1a), while that of the original Aztec solver on ES2 is 0.15 GFlops/PE with VOR=80%. As expected, the speed up was achieved largely due to the change of the matrix storage format that greatly helps the speed-up of matrix-vector product calculations in the sparse matrix solver. Additionally, exclusions or modifications of many conditional branches equipped for the general-purpose code also contribute to the speedup considerably. Figure1 shows the scalability of the new solver of TOUGH2-MP on the ES2. In addition to the two problems shown below in this paper (SPE10 in section 3.1 and DDC in section 3.2), two larger problems (Tokyo Bay [13] and QLASTIC [14]) of 25 to 30 million dof (degree of freedom) are also included. It is generally seen that the larger the model (dof), the better the scalability due to the relative load balance of computation and communication. For smaller models, the load of communication among PEs is more pronounced comparing to that of computation (and vice versa). Through the process of the solver improvement, it was also recognized that successful improvement of the solver results in faster computational speed but also worse scalability apparently. This is the reason that the scalability on ES2 is not better than that on T2K, as shown below.

In Figure 2, a scalability of TOUGH2-MP on T2K is presented for the Tokyo Bay case with a 10 million-grid model (30 million dof) [13] examined for the first 50 time steps. We gained “super-linear” speedup up to 512 PEs for the problem size. Figure 2 (right) compares the computation times for solving the same problem on ES2 and T2K. It should be noted that the theoretical peak performance of PE on ES2 is more than ten times faster than that of T2K (102.4G and 9.2GFlops respectively), however it is remarkable that the computation time with 16 vector processors on ES2 is nearly the same as or rather faster that with 512 scalar processors on T2K.



(a) MFLOPS/PE (b) GFLOPS/TOTAL

Figure 1 Computation performance of the new solver of TOUGH2-MP on The Earth Simulator 2. In addition to the two problems in this paper (SPE10 in section 3.1 and DDC in section 3.2), two larger problems (Tokyo Bay [13] and QLASTIC [14]) are also included. PE stands for "processing element" (i.e., processor).

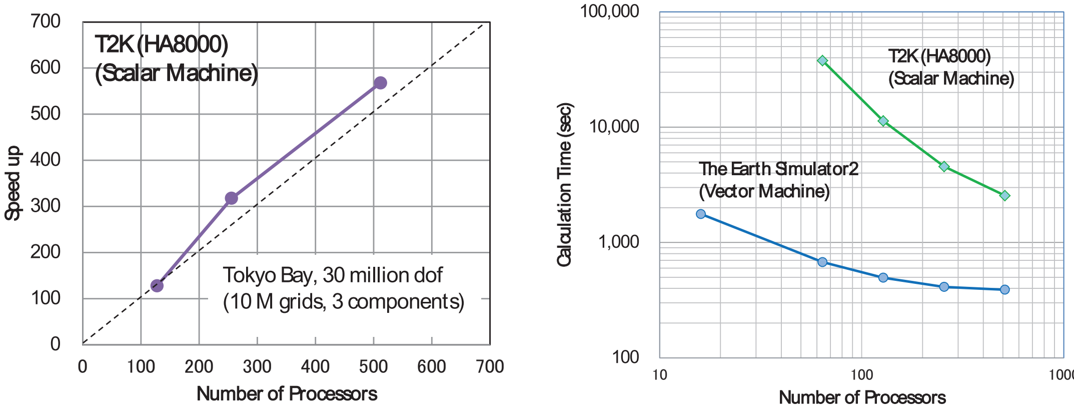


Figure 2 Scalability of TOUGH2-MP on T2K Open Supercomputer System exhibiting "super-linear" speed-up (left). The right figure shows comparison of computation time on ES2 and T2K for a 10 million-grid simulation at Tokyo Bay [13] for the first 50 time steps (right). Note that the theoretical peak performance of one PE on ES2 is more than 10 times faster than that on T2K (102.4G and 9.2GFlops respectively).

3. Numerical Simulation of CO_2 Behaviors in Deep Reservoirs

Here, we investigate effects of grid resolution on the two topics: 1) CO_2 behaviors in highly heterogeneous reservoirs; 2) the diffusion-dissolution-convection process that may cause gravity instability that greatly enhances the convective mixing of dissolved CO_2 in reservoirs in long-term.

3.1 CO_2 Behaviors in Highly Heterogeneous Reservoirs

Reservoir formations for storing CO_2 are usually regarded as heterogeneous porous media, often consisting of alternating sand and mud layers having quite different permeability and porosity. Obviously, because CO_2 preferentially migrates into higher permeable portion in the reservoir, the heterogeneity of reservoirs should be properly considered and represented in simulation models. However, it is well known that transient simulation of multi-phase flow in heterogeneous media generally requires very long computational time, because the heterogeneity of hydraulic properties strongly limits the length of time steps, resulting in a huge number of time steps to be solved in the simulation. As a practice in such as oil and gas industries, for performing simulations in a practically reasonable time, the heterogeneity is spatially averaged with reducing number of grid cells of the computation model (i.e., up-scaling). In this study, with the help of high-performance computing, we directly solved a highly heterogeneous reservoir model without such simplifications. Figure 3 shows the heterogeneous model known as SPE-10 model [9], representing irregular nature of sand/shale distribution in a reservoir with 1.122×10^6 ($60 \times 220 \times 85$) grid cells in the dimension of 6400m × 8800m × 170m. In this simulation, supercritical CO_2 is injected at the injector with the rate of 390 k tons / year, with producing brine groundwater with the rate of 580 k tons / year [10]. The distribution of CO_2 after 20-years injection is shown in Figure 4 (middle). For a comparison, a simulation result obtained from a homogeneous model with a unique average permeability and porosity is also shown (Figure 4, left). Because the density of supercritical CO_2 is smaller than that of groundwater, injected CO_2 tend to overrides on denser groundwater. In the homogeneous model, the override effect is prominent and the lower part of the reservoir volume cannot effectively be used for storing CO_2. The CO_2 plume spread widely on the top of the reservoir, suggesting higher risks of CO_2 leakage through undetected high-permeable features such as faults. On the other hand, in the heterogeneous model, CO_2 tends to migrate in sand portions with higher permeability, suppressing the gravity override. The more tortuous flow paths of CO_2 in the heterogeneous model results in larger contact area of CO_2 and groundwater, and thus enhances the dissolution of CO_2 in groundwater, which is deemed as more stable form of the storage than buoyant supercritical CO_2 plume. Figure 4 includes the change of CO_2 storage status in the reservoir over time. The dissolution of CO_2 in groundwater is enhanced nearly double in the heterogeneous model than that in the homogeneous model.

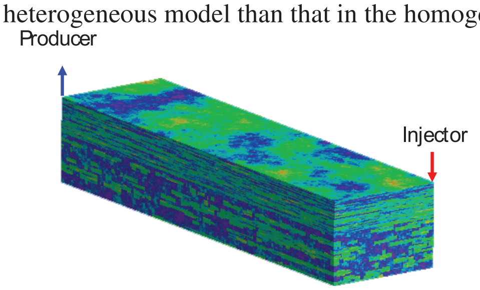


Figure 3 The SPE-10 model, a highly heterogeneous reservoir model. The colors indicate porosity of the sand and mud in the reservoir. The CO_2 injector and the water producer in the simulation are shown in the figure [10].

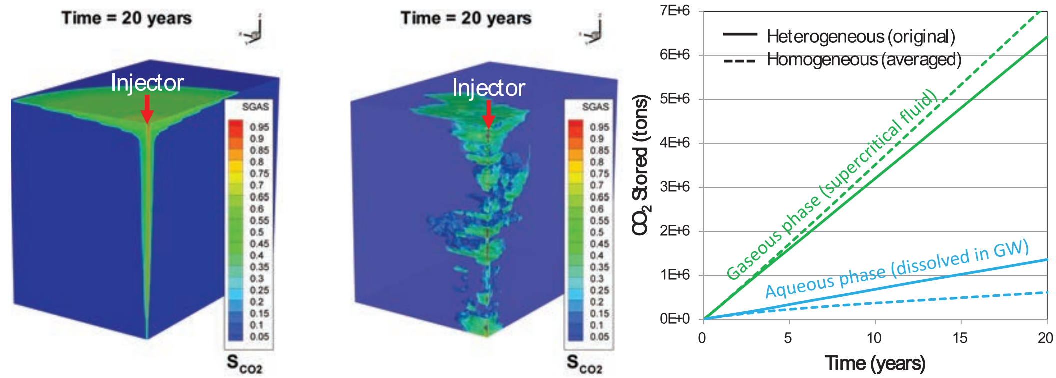
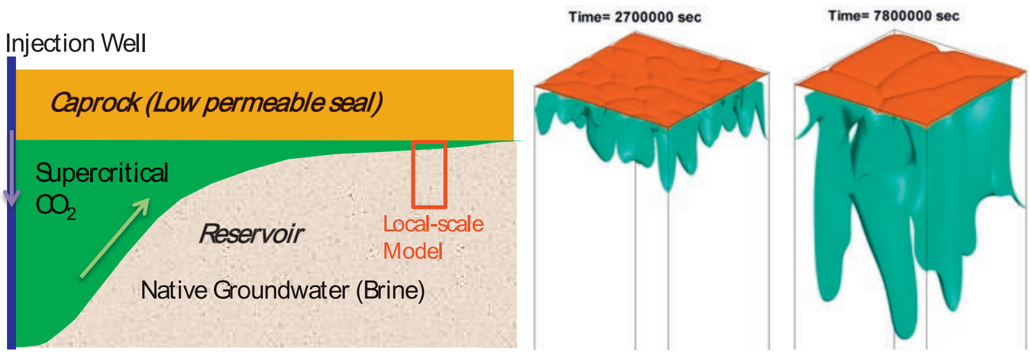


Figure 4 CO_2 plume spreading from the injector in the homogeneous (left) and heterogeneous model (middle). Time evolution of the CO_2 form stored in the reservoir (right). S_{CO2}: saturation of gaseous CO_2.

3.2 Diffusion-Dissolution-Convection Process of CO_2-Brine System

As mentioned above, injected supercritical CO_2 generally tends to override over native groundwater in the reservoir (Figure 5a). However, the supercritical CO_2 on top gradually dissolves in surrounding groundwater, and increases its density. This results in a situation that denser fluid laid on lighter fluid as schematically shown in the red-box in Figure 5a. In a certain time, the Rayleigh-Taylor instability invokes convective mixing of the groundwater [11]. The mixing would significantly enhance the CO_2 dissolution into groundwater, and reduce the amount of CO_2 in buoyant supercritical state, and eventually attain more stable storage. The simulation of the Rayleigh-Taylor instability is sensitive to numerical errors. The simulation grids should be fine enough to resolve incubation times for onset of convection, and spatial evolution of convective fingers or tongues [11][12]. Figure 5b shows a simulation result for a local-scale model of a small region (1m×1m×4m) with 1cm spacing, resulting in about 4 million gridblocks [12]. Starting from the initial condition that supercritical CO_2 is stagnate on the top of groundwater, CO_2 gradually dissolves in groundwater, developing a thickness of a CO_2 diffuse layer. When the thickness of the diffusive layer reaches a critical thickness, the convection with developing downward fingers of high-CO_2 water occurs. Massively parallel computation would make it possible to simulate not only the local process shown above, but also the whole system in reservoir scales (i.e., more than hundreds to thousands of meters) on the resolution of centimeter-scale grids. Figure 6 shows a preliminary simulation result performed for a homogeneous and horizontal reservoir model of 10km radius and 40m thickness. The model is finely discretized with about 10cm grid spacing. We successfully simulated the evolution of the convectional mixing process in entire reservoir, showing that the fingering gradually developed from centimeter to tens of meters scale enhancing the dissolution of CO_2 in groundwater, and the CO_2 in supercritical state stay on the top of the reservoir was eventually lost.

Figure 7 compares the result obtained from two models of 'coarse' and 'fine' grid-spacing. In the 'coarse' model, the grid-spacings in vertical and lateral direction are both increased 10 times from the original 'fine' model shown above. In Figure 7a, the supercritical CO_2 laid along the reservoir top is recognized as the red colored portion of high CO_2 mass fraction in aqueous phase. It was seen that the coarseness of the grid artificially stabilizes the layer of CO_2-saturated groundwater on the top [11]. Figure 7b shows that the coarse model underestimates the dissolution of CO_2 by almost half, and thus underestimates the long-term stability of CO_2 stored in the underground reservoir. Usually 3D field scale simulations employ grid model with the size of tens to hundreds of meters, but finer grid model will be required to predict the long-term fate of CO_2 appropriately.



(a) Local-scale model (b) Simulation results

Figure 5 (a) The concept of the local-scale model and (b) the simulated results of CO_2 concentration dissolved in groundwater. The model size is 1m×1m×4m. The iso-surfaces in the right figures are colored for CO_2 mass fractions (brown: 0.025, green: 0.008）

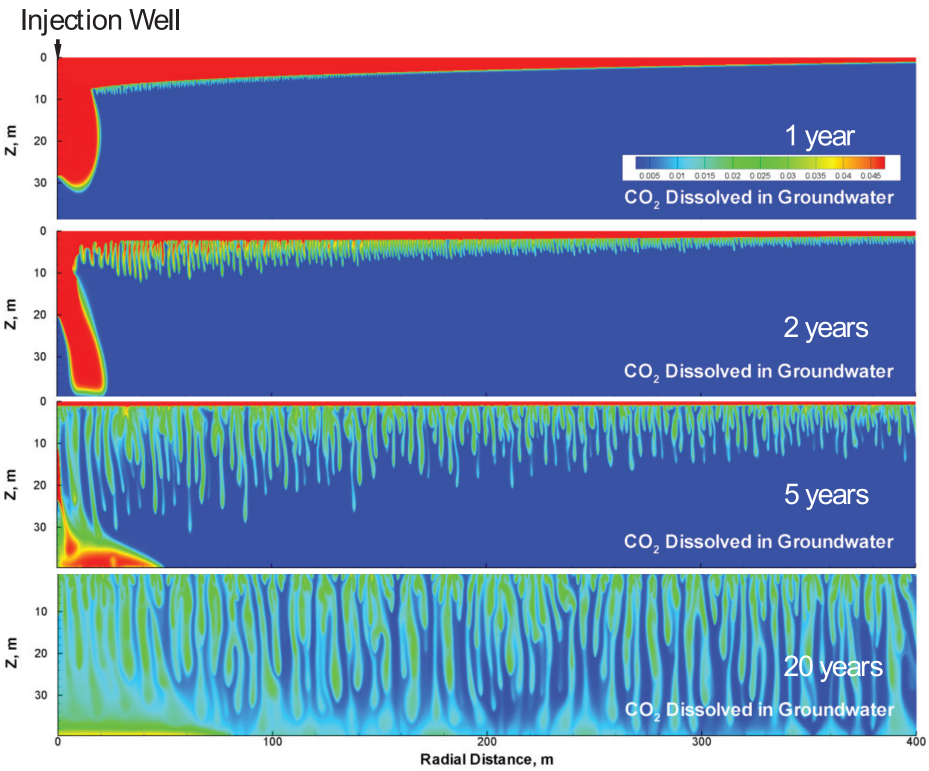
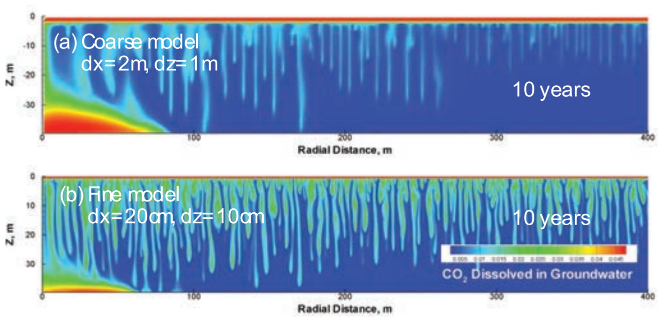
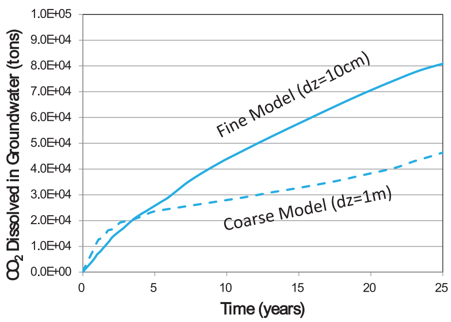


Figure 6 A preliminary simulation result of the diffusion-dissolution-convection process in a radially symmetric homogeneous model at a reservoir-scale (10km radius and 40m thickness). CO_2 is injected in supercritical state with the rate of 100k tons/year for one year. The contours show the time evolution of CO_2 mass fraction in the aqueous phase (groundwater) in the post-injection period. Due to the gravity convection, the supercritical CO_2 which has overridden over groundwater during the injection period is dissolved promptly, and eventually disappears (completely dissolved in the groundwater). The permeability and porosity are 1darcy and 20% respectively, employing the Corey equation for relative permeability and neglecting capillarity.



(a) CO_2 mass fraction in the aqueous phase at 10 years



(b) CO_2 dissolved in groundwater over time

Figure 7 Impact of grid spacing on the prediction of long-term CO_2 dissolution in groundwater.

4. Concluding Remarks

A general purpose hydrodynamics code TOUGH2-MP exhibits excellent performance and scalability after adequate tune-ups of the code on the Earth Simulator2 and T2K supercomputer. The efficiency in parallelization is enough to utilize hundreds to thousands of processors, so that we are capable of solving a reservoir model with multi-million gridblocks in a practical time. At present, it is suggested that the well-tuned code on the vector machine runs 1 to 2 orders faster than the original version on the scalar massive cluster, but there is still room of further optimization on the latter.

Using the code and the supercomputers, grid resolution effects were investigated for the following two examples: 1) CO_2 behaviors in highly heterogeneous reservoir formations; 2) the diffusion-dissolution-convection process that may cause gravity instability greatly enhancing convective mixing of dissolved CO_2 in reservoirs in long-term. These simulations illustrate the practical necessity of fine grid-resolution in numerical reservoir models, and thus importance of high-performance computing for predicting the behavior and fate of CO_2 even in actual storage projects in the future.

Acknowledgements

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