Numerical Simulation of Long-Term Fate of CO_2 Stored in Deep Reservoir Rocks on Massively Parallel Vector Supercomputer

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Abstract. As one of the promising approaches for reducing greenhouse-gas content in the atmosphere, CCS (carbon dioxide capture and storage) has been recognized worldwide. CO_2 is captured from large emission sources and injected and stored in deep reservoir rocks, including saline aquifers, depleted oil and gas field. Under typical pressure and temperature conditions at deep reservoirs (depths > 800m), CO_2 will be stored in supercritical state, subsequently dissolving in groundwater, and eventually forming carbonate minerals through geochemical reactions in a long-term (e.g., thousands of years). To ensure the safety and permanence of the storage, numerical simulation is considered as the most powerful approach for predicting the long-term fate of CO_2 in reservoirs. A parallelized general-purpose hydrodynamics code TOUGH2-MP has been used on scalar architectures where it exhibits excellent performance and scalability. However, on the Earth Simulator (ES2), which is a massively parallel vector computer, extensive tune-ups were required for increasing the vector operation ratio. In this paper, the performance of the modified TOUGH2-MP code on ES2 is presented with some illustrative numerical simulations of long-term fate of CO_2 stored in reservoirs.

Keywords: CCS, Hydrodynamics, Vector processors, The Earth Simulator.

1 Introduction

CCS (carbon dioxide capture and storage) is an emerging and promising technology for reducing greenhouse-gas content in the atmosphere, through capturing CO_2 from large emission sources and injecting and storing it into deep reservoir rocks, including saline aquifers, depleted oil and gas field [1]. Under typical deep reservoir conditions (depths > 800m), CO_2 will be stored in supercritical state, subsequently dissolving in

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groundwater, and eventually forming carbonate minerals through geochemical reactions in a long-term (e.g., hundreds to thousands of years). Numerical simulation is regarded as the most powerful approach for predicting the long-term fate of CO_2 in reservoirs, to ensure the safety and permanence of the storage. The simulations are generally conducted by using numerical simulators of multi-component, multi-phase fluid flow in porous media, but can often be computationally demanding for large-scale, high-resolution models because of complex non-linear processes involved.

In this study, we implemented a hydrodynamics code TOUGH2-MP on a massively parallelized vector computer, the Earth Simulator (ES2) in Japan. The code was extensively modified for the vector computer including the replacement of the original matrix solver to another suitable for vector processors. This paper presents the performance of the improved code on ES2 for high-resolution simulations of CO_2 behavior in deep reservoirs on the following two topics 1) CO_2 migration in highly heterogeneous geologic formations; 2) DDC (dissolution-diffusion convection) process in CO_2 – brine system, which are both important for predicting long-term fate of CO_2 stored in reservoirs.

2 General-Purpose Flow Simulator TOUGH2-MP

TOUGH2 [2] is a general-purpose numerical simulator for multi-dimensional fluid and heat flows of multiphase, multicomponent fluid mixtures in porous and fractured media. TOUGH2 solves mass and energy balance equations that describe fluid and heat flow in multiphase, multicomponent systems.

$$\frac{d}{dt}\int_{V_n} M^\kappa \, dV_n = \int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} \, d\Gamma_n + \int_{V_n} q^\kappa \, dV_n \tag{1}$$

where, M^κ: energy or mass of component κ (e.g., water, CO_2, NaCl) per volume, $\mathbf{F}^\kappa$: mass or heat flux, q^κ: sink and sources, $\mathbf{n}$: normal vector on the surface element $d\Gamma_n$ pointing inward into V_n. The mass accumulation term in the left hand side is,

$$\text{Mass:} \quad M^\kappa = \phi \sum_\beta S_\beta \rho_\beta X_\beta^\kappa \tag{2}$$

$$\text{Heat:} \quad M^h = (1-\phi)\rho_R C_R T + \phi \sum_\beta S_\beta \rho_\beta U_\beta \tag{3}$$

where, ϕ: porosity, S_β: the saturation of phase β, ρ_β: the density of phase β, X^κ_β: the mass fraction of component κ present in phase β, ρ_β: grain density, T: temperature (°C), C_R: specific heat of the rock, U_β: specific internal energy of phaseβ.

Fluid advection is described with a multiphase extension of Darcy's law.

$$\mathbf{F}_\beta = \rho_\beta \mathbf{u}_\beta = -k \frac{k_{r\beta}\rho_\beta}{\mu_\beta} \left(\nabla P_\beta - \rho_\beta \mathbf{g} \right) \tag{4}$$

Here $\mathbf{u}_\beta$ is the Darcy velocity (volume flux) in phase β, k is absolute permeability, $k_{r\beta}$ is relative permeability to phase β, μ_β is viscosity, and P_β is the fluid pressure in phase

β (=P+$P_{c\beta}$, $P_{c\beta}$: the capillary pressure). The $k_{r\beta}$ and $P_{c\beta}$ are normally given as a non-linear function of saturation S_β, which is subject to change at each time step of transient simulations.

Heat flux includes conductive and convective components

$$\mathbf{F}^{h} = -\lambda \nabla T + \sum_{\beta} h_{\beta} \mathbf{F}_{\beta} \tag{5}$$

where, λ is thermal conductivity, and h_β is specific enthalpy in phase β.

Space discretization is made directly from the integral form of the basic conservation equations, without converting them into partial differential equations (IFDM, integral finite difference method). Time is discretized fully implicitly as a first-order backward finite difference.

$$\begin{aligned} &R_n^{\kappa}(\mathbf{x}^{t+1}) = M_n^{\kappa}(\mathbf{x}^{t+1}) - M_n^{\kappa}(\mathbf{x}^{t}) \\ &-\frac{\Delta t}{V_n}\left\{\sum_m A_{nm} F_{nm}^{\kappa}(\mathbf{x}^{t+1}) + V_n q_n^{\kappa,t+1}\right\} = 0 \end{aligned} \tag{6}$$

where, $\mathbf{x}^t$: the independent primary variables (i.e., pressure, temperature, saturation …) at time step t, R^{κ}_n: the residuals, M^{κ}_n: mass or heat accumulation term averaged over the element (gridblock) n with volume V_n, Δt: time step length, F_{nm} is the average value of the (inward) normal component of flux $\mathbf{F}$ over the surface segment A_{nm} between volume elements V_n and V_m. The equations (6) can be iteratively solved by Newton/Raphson method.

ECO2N [3] is a fluid property (EOS, equation of state) module designed for applications to geologic CO_2 storage, including a comprehensive description of the thermodynamics and thermophysical properties of H_2O-NaCl-CO_2 mixtures, modeling single and/or two-phase isothermal or nonisothermal flow processes, two-phase mixtures, fluid phases appearing or disappearing, as well as salt precipitation or dissolution. The nonlinear processes include interactions of immiscible multi-phase fluids in porous media; thermo-physical properties of supercritical CO_2 fluid that can changes rapidly against the pressure and temperature conditions at reservoir depths.

In this study, we use a parallel simulator TOUGH2-MP [4] with ECO2N fluid property module, which is a three-dimensional, fully implicit model that solves large, sparse linear systems arising from discretization of the partial differential equations for mass and energy balance. The original TOUGH2-MP uses MPI for parallel implementation, the METIS software package [5] for simulation domain partitioning, and the iterative parallel linear solver package Aztec [6] for solving linear equations by multiple processors. On scalar architecture machines, it exhibits excellent performance and scalability. In fact, “super-linear speedup” meaning speedup higher than expected linear speed up (a speedup of more than *p* when using *p* processors) has been reported on multi-core PCs [4].

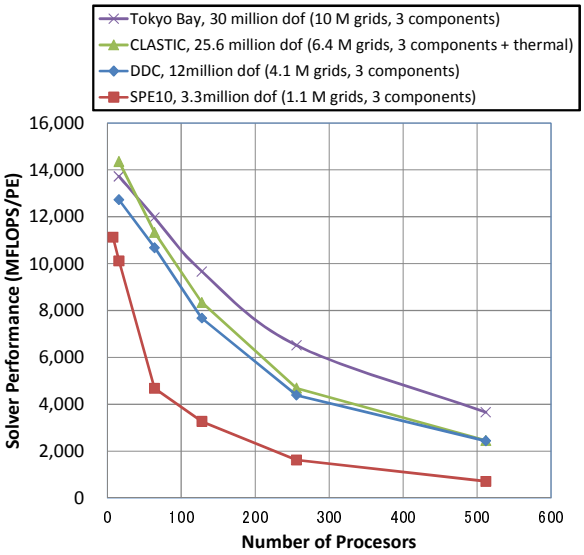
3 Code Implementation and Modification on ES2

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 processors 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.

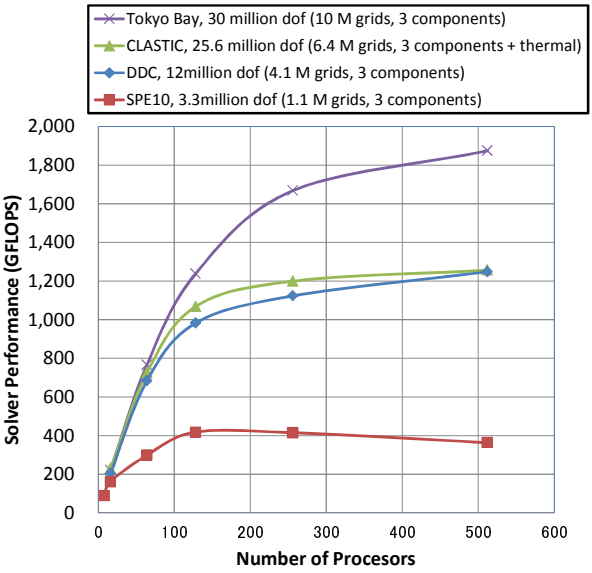
TOUGH2-MP was ported to the Earth Simulator, but a special tune-up to increase its vector operation ratio (VOR) was needed for the efficient use of the ES vector processors. The original source code of TOUGH2-MP over 40,000 lines was originally written assuming the use on scalar computers. Thus it contains 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 another matrix solver that employs DJDS format. The solver was found among GeoFEM [8], which has been implemented and optimized for various types of parallel computers, from PC cluster to the Earth Simulator. In addition, we performed loop-unrolling and inline expansion wherever possible and effective, and rewrote bottleneck computations (loops) in the fluid property (EOS) module.

On ES2, the modified code is about 60 times faster than the original code with Aztec solver. The speed of the new solver 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.



(a) MFLOPS/PE



(b) GFLOPS/TOTAL

Fig. 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 4.1 and DDC in section 4.2), two larger problems (Tokyo Bay [13] and QLASTIC [14]) are also included.

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 4.1 and DDC in section 4.2), two larger problems (Tokyo Bay [13] and QLASTIC [14]) are also included. The solver performance is considerably reduced with increasing number of PEs probably because of the load increase of communication among PEs, which is pronounced for smaller models (i.e., SPE10).

4 Numerical Simulation of CO_2 Behaviors in Deep Reservoirs

This study intends to demonstrate potential benefits from high performance computing for simulating CO_2 behavior in deep reservoirs for important scientific and engineering topics. Here, we investigate uncertainties due to grid resolution effects on the two topics: 1) CO_2 behaviors in highly heterogeneous reservoir formations; 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.

4.1 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 of 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 2 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, CO_2 in supercritical state 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 3. For a comparison, a simulation result obtained from a homogeneous model with a unique average permeability and porosity is also shown. 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. In addition, 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

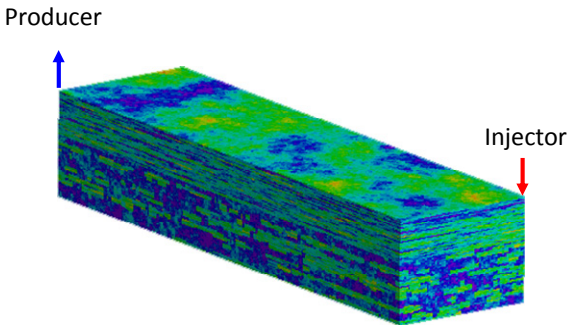


Fig. 2. SPE-10 model, a highly heterogeneous reservoir model. The colors indicate porosity of the sand and mud in the reservoir. The CO_2 injector and the water producer used in the simulation are shown in the figure [10].

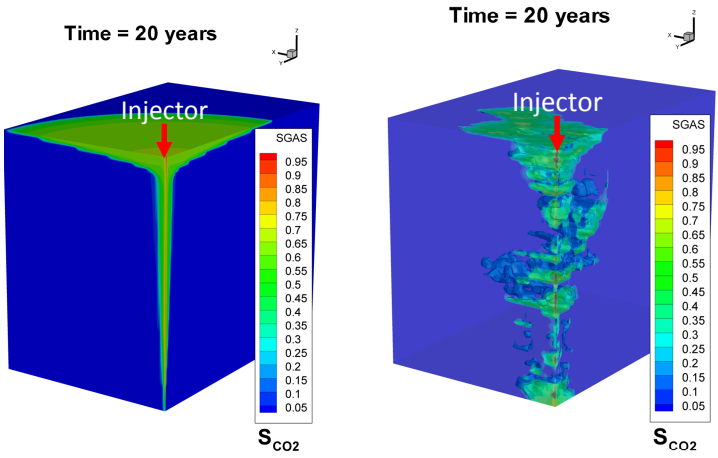


Fig. 3. CO2 plume spreading from the injector in the homogeneous (left) and heterogeneous model (right). S_{CO2}: saturation of gaseous CO_2.

deemed as more stable form of storage than buoyant supercritical CO_2 plume. Figure 4 includes the change of CO_2 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.

As seen in the above, although the heterogeneity of reservoir is an important key in predicting the efficiency and risks of CO_2 storage, two-phase flow simulations in heterogeneous porous media computationally demanding in general. The 20-years simulation of the homogeneous model was finished only in about 3 node-hours (about 650 time steps), while it took more than 900 node-hours (about 40,000 time-steps) for the heterogeneous model. The simulation was performed by using 2 or 4 nodes (16 to 32 PE) of ES2, taking into account the limited scalability for this SPE10 model as shown in Figure 1.

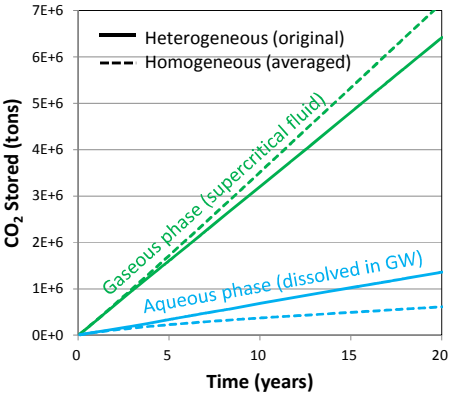


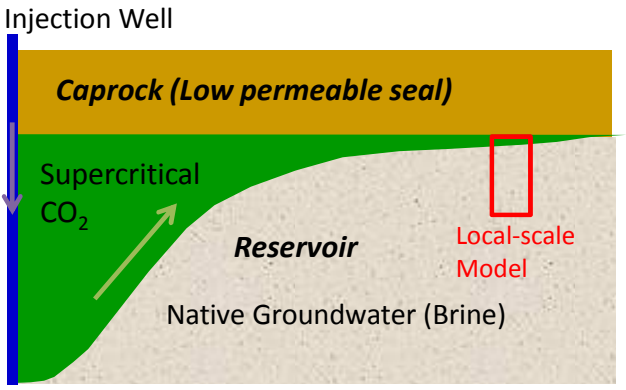
Fig. 4. Time evolution of the CO_2 form stored in the reservoir

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

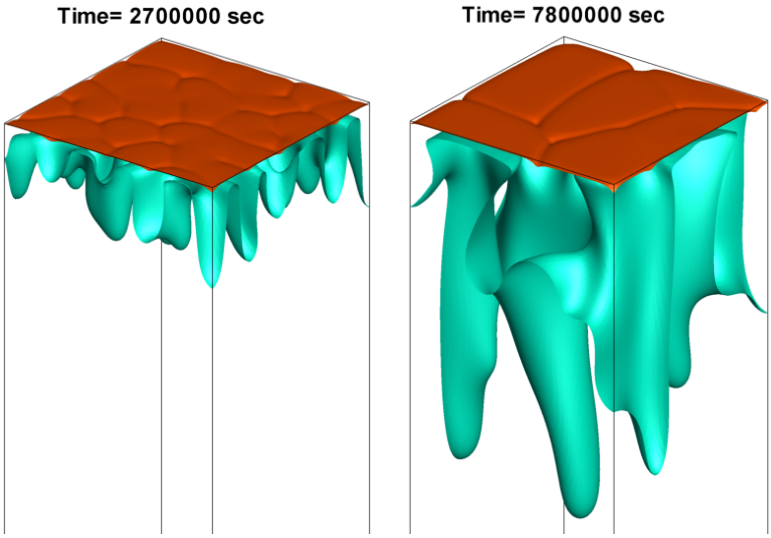
As mentioned above, injected supercritical CO_2 generally tends to override over native groundwater in the reservoir (Figure 5a). The supercritical CO_2 on top gradually dissolves in surrounding groundwater, and increases its density. This results in a situation that denser fluid laid on lighter fluid 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.



(a) Local-scale model



(b) Simulation results

Fig. 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).

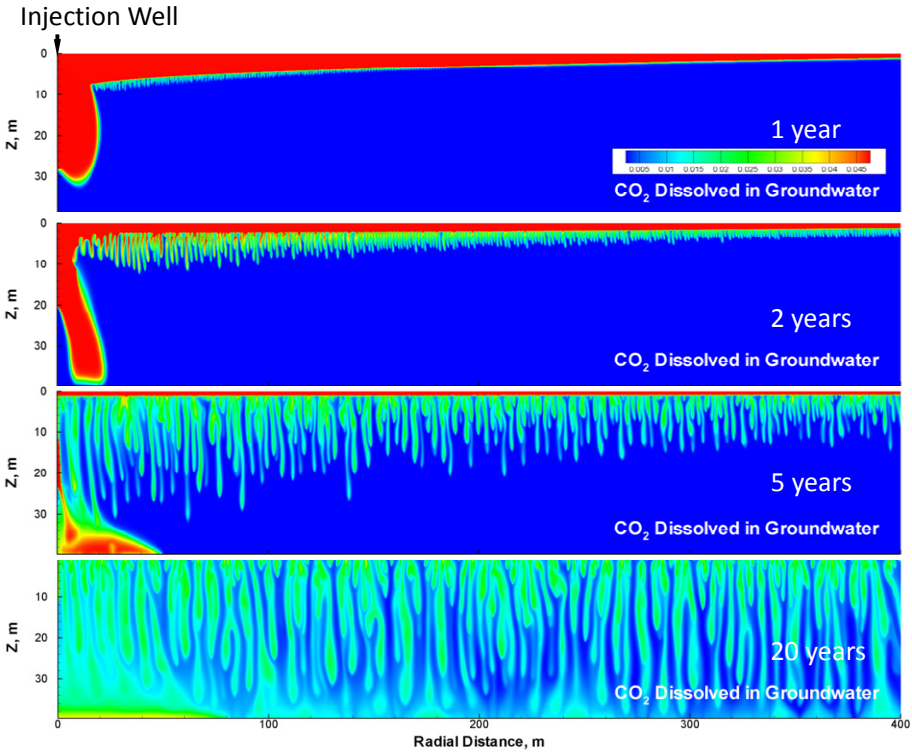
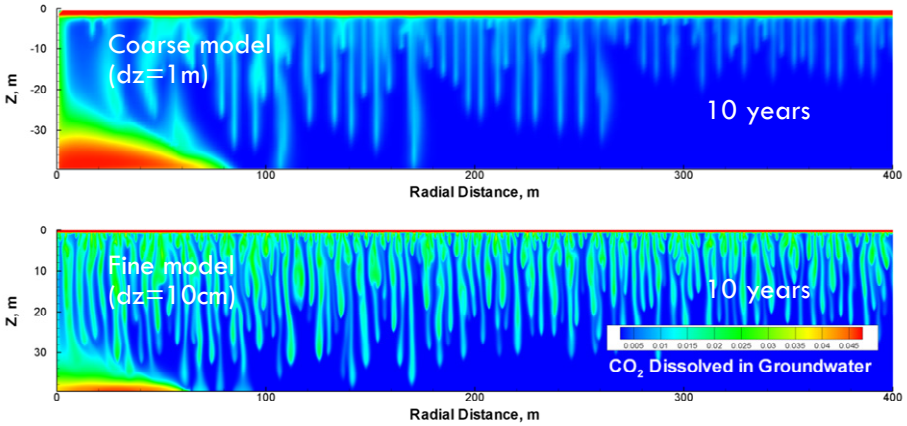
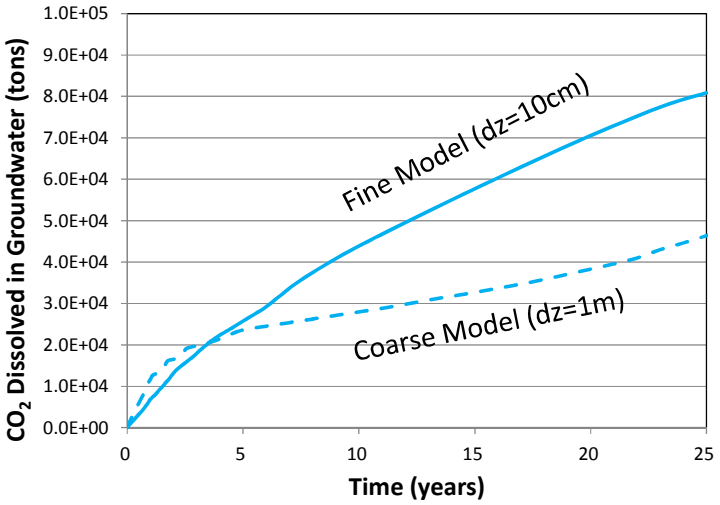


Fig. 6. A preliminary simulation result of the diffusion-dissolution-convection process in a radially symmetric homogeneous model at a reservoir-scale (10km radius and 40m thickness). CO_2 is injected in supercritical state with the rate of 100k tons/year for one year. The contours show the time evolution 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.

Figure 7 compares the result obtained from two models with different grid-spacings. 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 the time evolution of the amount of CO_2 dissolved in groundwater. It is seen that the rough 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



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



(b) The time evolution of the amount of CO_2 dissolved in groundwater

Fig. 7. Impact of grid spacing on the prediction of CO_2 dissolution in groundwater

to hundreds of meters, but finer grid model will be required to predict the long-term fate of CO_2 appropriately.

These above simulations were both performed by using 2 to 16 nodes (8 to 128 PE) of ES2. Vector efficiency was observed in the same level as in other measurements.

5 Conclusion

A general purpose hydrodynamics code TOUGH2-MP was successfully implemented on the Earth Simulator (ES2). The performance of the TOUGH2-MP code on ES2 was considerably improved by the efforts including (1) the replacement of matrix solver and (2) restructuring and rewriting of the EOS routines. So far, the computational performance of 10 to 14 GFlops/PE (approximately 10-14% of peak performance of a vector processor on ES2 with a vector operation ratio > 99.5%) has been achieved. The achieved performance is satisfactory for the general purpose code, which was originally developed for scalar architectures, but not for vector architectures.

Using the code, uncertainties due to grid resolution effects on the two topics were investigated: 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 long-term fate of CO_2 even in actual storage projects in the future.

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