Massively parallel simulation of Geologic CO\textsubscript{2} storage on the Earth Simulator

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Abstract
CCS (carbon dioxide capture and storage) is a promising approach for reducing the greenhouse gas content in the atmosphere, through capturing carbon dioxide (CO\textsubscript{2}) from large emission sources and injecting it into reservoirs (such as deep saline aquifers). Large-scale storage projects will likely involve very long-term storage of huge amounts of CO\textsubscript{2}, potentially exceeding hundreds of millions of tonnes (Mt). This study intends to demonstrate potential benefits of massively parallel computing technology for simulating geologic CO\textsubscript{2} storage for important scientific and engineering topics. 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. After tune-ups of the code, TOUGH2-MP generally exhibits excellent performance, and we achieved computational performance of 10-14 GFlops/PE (i.e., approximately 10-14% of peak performance of ES2), which is considered to be satisfactory for the general purpose code. From last year, we are continuously performing a simulation of a diffusion-dissolution-convection process in a three-dimensional, field-scale reservoir model, which is largely computationally demanding; for investigating the impact of the convective mixing of dissolved CO\textsubscript{2} on long-term stability of CO\textsubscript{2} in storage reservoirs. In this year, the simulation for 1000 years has been completed.

Keywords: large-scale simulation, CCS, CO\textsubscript{2}, global warming, groundwater
Figure 1 A preliminary simulation result of diffusion-dissolution-convection process in a 3D reservoir model (for 1000 years after injection stopped). CO$_2$ is injected in supercritical state with the rate of 100kt/year for one year. Due to the gravity convection, CO$_2$ dissolution in groundwater is greatly enhanced and gradually the supercritical CO$_2$ disappears.