Application of Lagrangian Techniques to Evaluate Ocean Carbon Sequestration

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Abstract

Lagrangian models have been developed to simulate the transport of injected carbon dioxide using the predicted hydrodynamic field of an Eulerian (grid-based) ocean general circulation model (OGCM). Lagrangian simulation can better resolve the ecologically sensitive intermediate field ($10^2 \sim 10^5$ m), and thus bridge the gap between near-field plume models and coarsely-gridded OGCMs. Once injected carbon spreads sufficiently to be resolved by the OGCM grid, Eulerian concentrations can be calculated and long-term OGCM sequestration simulations can proceed with an improved initial condition. Alternatively, sequestration efficiency can be simulated using a Lagrangian model alone.

Evaluating Ocean Sequestration…

Evaluating the environmental feasibility of ocean carbon sequestration requires that two important questions be addressed:

- What environmental impacts will accrue to marine organisms?
- How effectively will the injected carbon be sequestered?

Adequately addressing these concerns requires simulation of injected carbon transport over a wide range of spatial and temporal scales. Currently, simulations are primarily being performed using two classes of models:

- Near-field models of injection site (typical domain ~ 100m)
  - integral plume models (e.g., Crounse *et al.*, 2001)
  - CFD codes (eg., Sato *et al*., 2001, Chen *et al*., 2001; Alendal and Drange, 2001)
- Far-field models of carbon transport
  - Ocean General Circulation Models (OGCMs)
    - o Basin scale (e.g., Marshall *et al.*, 1997)
    - o Global scale (e.g., Caldeira *et al.*, 2000)

Lagrangian Models

As a complement to the far field OGCMs, we are constructing Lagrangian models which can simulate carbon transport on scales beyond the near field. The main purpose for this work is to offer improved capabilities in resolving intermediate field carbon transport (Application I) and to offer a computationally efficient way to characterize sequestration efficiency on a large scale (Application II). The benefits of the Lagrangian approach in the evaluation of carbon sequestration are described in the application section of this presentation.

We are evaluating three different Lagrangian approaches in the development of our modeling framework:

1) random walk particle tracking
2) forward puff tracking
3) backward puff tracking

(1) Random Walk Particle Tracking

The injected carbon is represented by discrete mass particles which are advected by the ambient flow field and diffused by a random walk process, i.e., using first order integration:

$$\Delta \mathbf{x} = \mathbf{A}\,\Delta t + B\,\mathbf{Z}\sqrt{\Delta t}$$

$$\mathbf{A} = \mathbf{u} + \nabla \cdot E$$

$$BB^T = 2E$$

Δ**x**	= change in 3-D particle position in timestep Δt
A	= deterministic forcing vector:
B	= deterministic scaling matrix:
U	= 3-D velocity vector
E	= tensor of diffusivities
Z	= vector of 3 independent random variables (μ=0; σ^2=1)

(2) Forward Puff Tracking

Injected mass is represented as an ensemble of "puffs" that are injected at fixed time intervals, and whose centers of mass are advected by the flow field and whose dimensions grow according to a predefined relative diffusion law (e.g., one based on observations):

$$\Delta x_c = u \Delta t \qquad \sigma^2 = \sigma_0^2 + \int_0^t 2E \, d\tau$$

Each puff represents a Gaussian concentration distribution where the peak concentration is located at the center of the puff $\{x_c, y_c, z_c\}$:

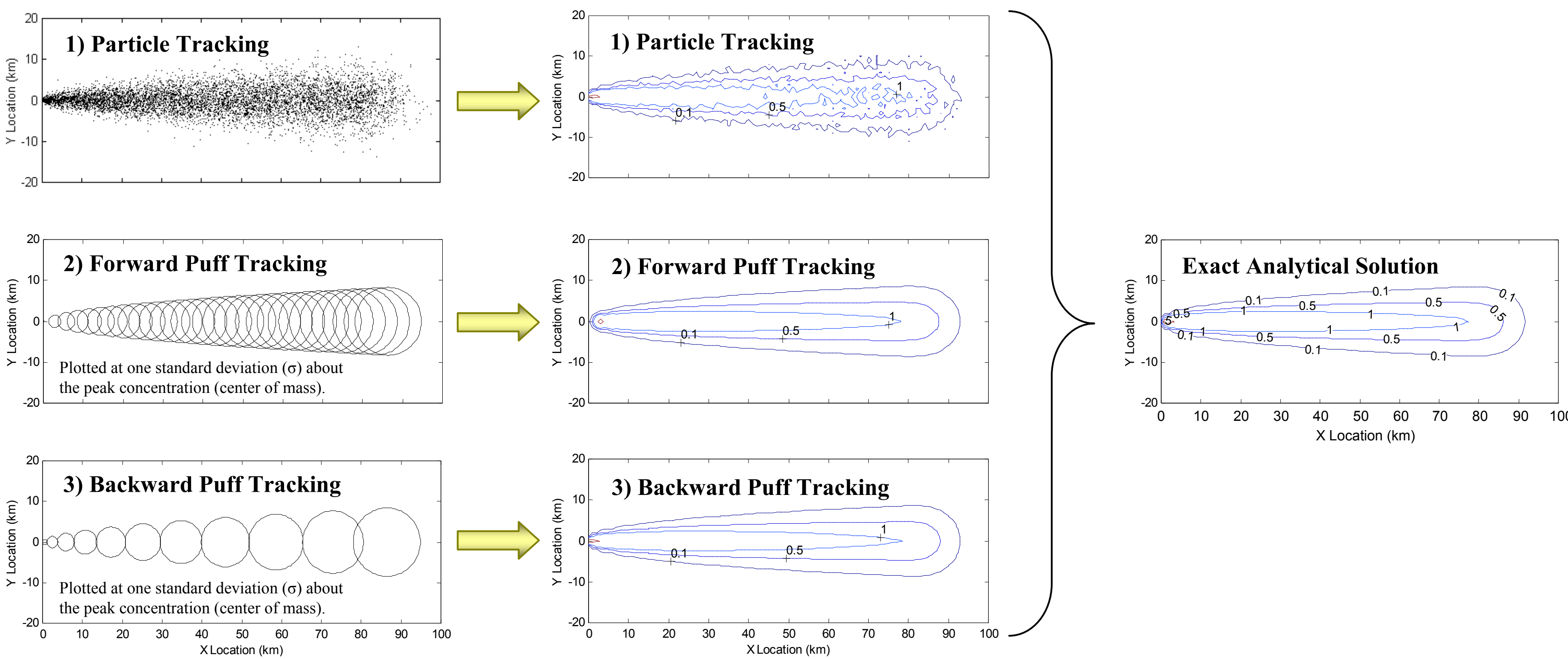
$$C(x,y,z) = \frac{M}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp\left(-\frac{(x-x_c)^2}{2\sigma_x^2} - \frac{(y-y_c)^2}{2\sigma_y^2} - \frac{(z-z_c)^2}{2\sigma_z^2} \right)$$

(3) Backward Puff Tracking

The method is similar to forward puff tracking, except plume concentrations are completely reconstructed at each output time by mapping puffs backward in time. Fewer puffs are usually required because the time interval represented by each puff is varied to achieve an optimal spatial spacing between puffs.

Lagrangian Source Representation

Below are simulation results of a 2D plume in a unidirectional current with homogeneous diffusion. The test case demonstrates how the plume is represented in each of the three techniques (left column). A square counting grid of 1 km resolution was used to convert particle densities to concentrations. Concentration contours have been generated for each of the methods, as shown in the three figures in the middle column. The predicted concentration contours for each method match the analytical solution (right) for this simple test case, provided a sufficient number of particles or puffs are used.

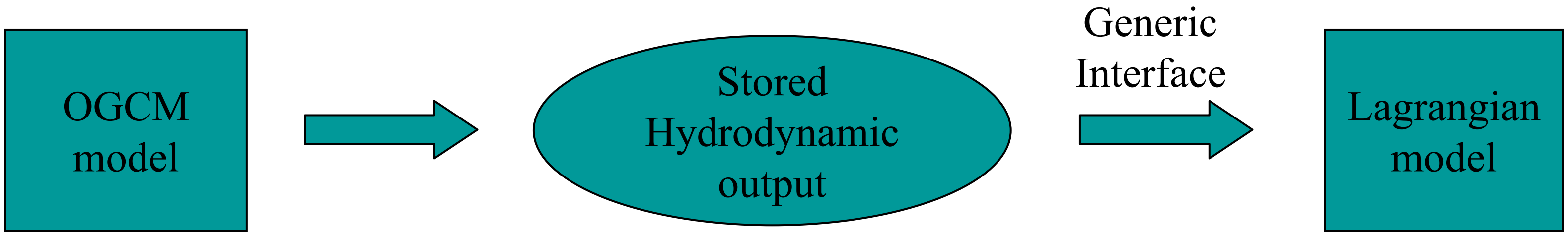


Efficiency vs Accuracy

The three methods have tradeoffs regarding efficiency vs accuracy. For simple domains and flow fields such as the case presented above, the puff methods are much more computationally efficient than particle tracking. Unlike the puff methods, the particle tracking method does not generate smooth concentration contours (although the smoothness increases with an increasing number of particles). However, the puff methods lose accuracy in cases of large spatial variability in ambient currents or diffusivity, and are therefore not as generally applicable as the particle tracking method.

Interfacing with OGCMs

The Lagrangian methods rely on interpolating hydrodynamic fields that have been generated by a parent hydrodynamic model (OGCM). The accuracy of the Lagrangian prediction is obviously dependent on the grid resolution of the parent OGCM. For the models to be effectively used in the evaluation of many different potential injection sites, it is important that they can interface with the most appropriate (finely resolved) OGCM. We are therefore designing the OGCM interface to be as generic as possible.



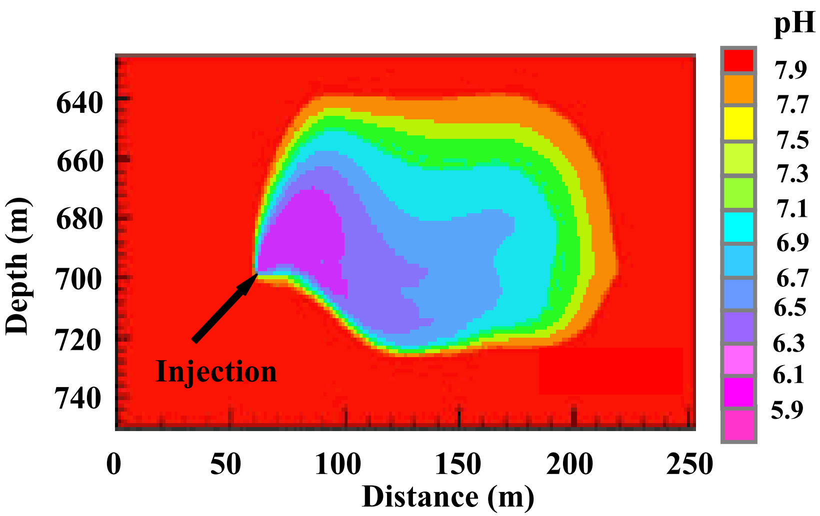
Application I
Improved Simulation of the Intermediate Field

Introduction

Near field models, including integral plume models (Crounse, 2001) and CFD codes (Sato *et al*., 1998; Chen *et al*., 2001; Alendal and Drange, 2001), have domains up to about 100m from the point of injection and are vital because they simulate the initial development and dilution of the injected carbon plume. For sequestration efficiency, the vertical extent of the plume (i.e., the trap height) dictates the ultimate fate of the injected carbon, and to evaluate impacts, especially acute impacts near the injection, one needs to understand the near field concentration distribution as well as the anticipated duration of organism exposure to these distributions. Beyond the near field, predictions are generally made using a numerical far field model, which can include basin scale or global OGCMs (Orr *et al*., 2001). In either case, the near field model provides the injection boundary condition: injected carbon is represented as an Eulerian (grid-based) concentration, allowing acute and chronic impacts beyond the near field to be analyzed. Sequestration efficiency can also be evaluated with the OGCM. Since the timescale of interest for carbon sequestration is hundreds of years, such calculations require that the OGCM domain must encompass the entire globe.

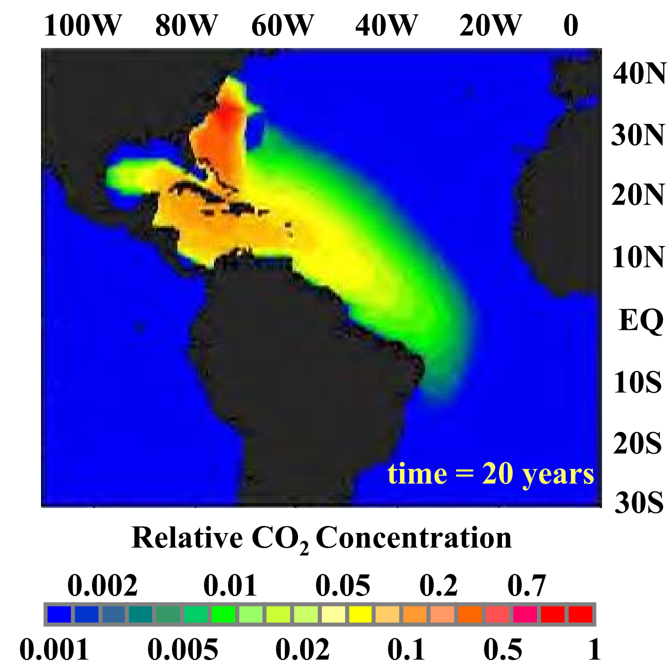
Existing Model Scale Disparity

Near field plume model of an injection site (Alendal, 2001). Typical domain scales for these models is ~ 10^2 m.



Scale Gap

OGCM simulation (LLNL) of a direct injection. Typically the domain scales are global, with horizontal resolution of $10^4 \sim 10^5$ m.

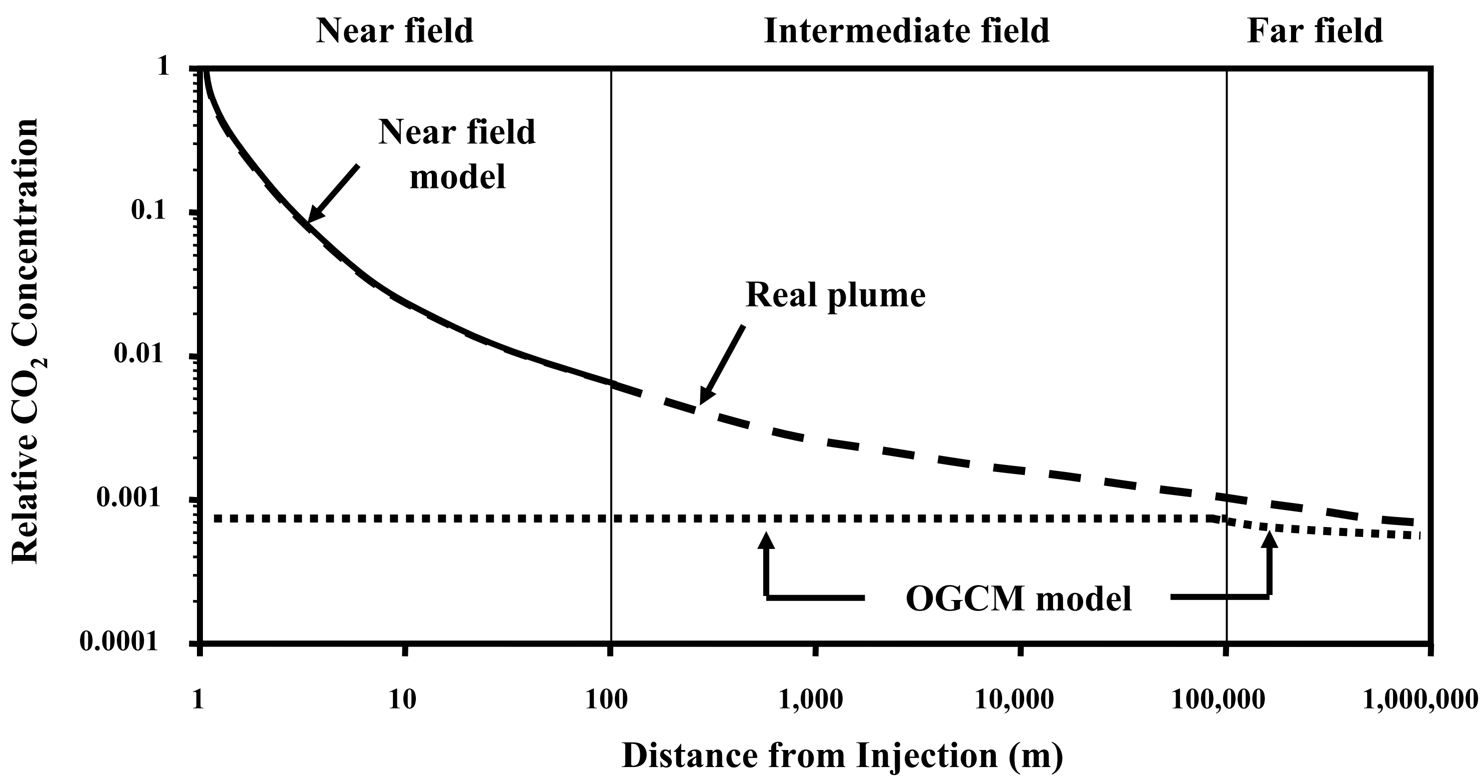


The large gap in scales between the domain of the near field model and the resolution of the far field model means that the spatial distribution of injected CO_2 in the intermediate field cannot be resolved by the OGCM grid.

Impacts of Scale Disparity

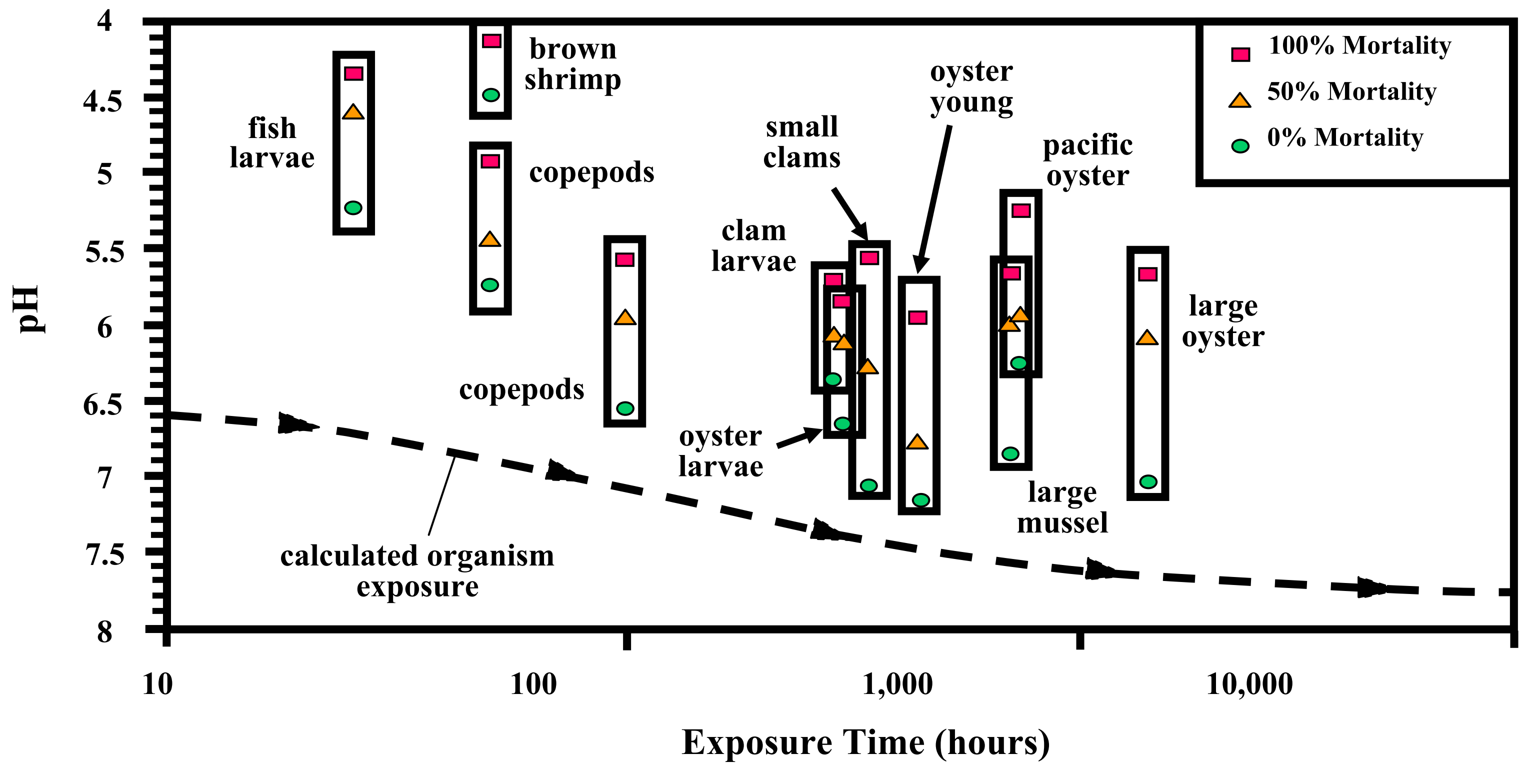
Two major consequences result from this scale disparity:

- The environmental impact will be under-predicted by the OGCM in the intermediate field.
- Long-term sequestration efficiency may be under-predicted as the near field plume will be spread both horizontally and vertically over a larger region.



Importance of the Intermediate Field

The figure below displays compiled biological mortality data (Auerbach *et al.*, 1997) due to changes in ambient pH under various exposure times. These data can be used in combination with simulated organism exposure to assess the stress under which an exposed organism is placed.

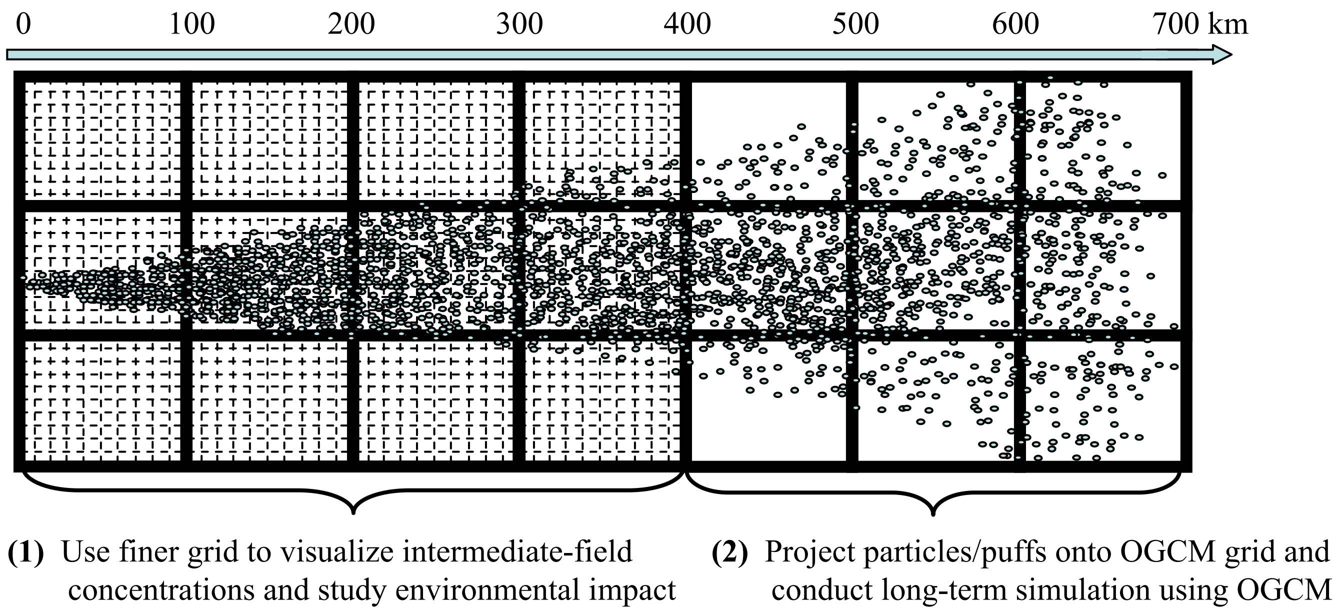


Importance of the Intermediate Field

To illustrate the importance of the intermediate field environmental impacts, the mean pH experienced by a passive organism floating along the centerline of a simple 2D plume is plotted (dashed line on preceding plot). The plume was calculated analytically (Brooks, 1960) and is representative of a 130 kg/s release of CO_2 (~ a 500 MW coal-fired plant) spread over 100 diffuser ports spaced 20 m apart in a steady 0.05 m/s current (u) with a plume height of 25 m. The exposure history is calculated assuming x = u * t. It is important to note that the organism comes closest to the mortality data in the 100 – 500 hour interval (10^5 – 10^6 s). In a current of 1-10 cm/s, the organism will have traveled ~ 10^3 to 10^5 m (i.e., the intermediate field) during this interval. The analysis suggests that understanding the intermediate field concentration distribution is crucial to assessing environmental impact.

How Can Lagrangian Models Be Used?

1) Environmental impact in the intermediate field can be better understood as more realistic concentration distributions can be visualized. The particle tracking model can be used to simulate the pH exposure history of passive organisms, which can be compared to mortality data.
2) Lagrangian models can bridge the scale gap between the near field and the far field by providing OGCM long-term sequestration efficiency simulations with a better injection boundary condition. Lagrangian models can simulate transport until the plume is adequately resolved by the OGCM grid.



Application II

Simulation of

Long-term Sequestration

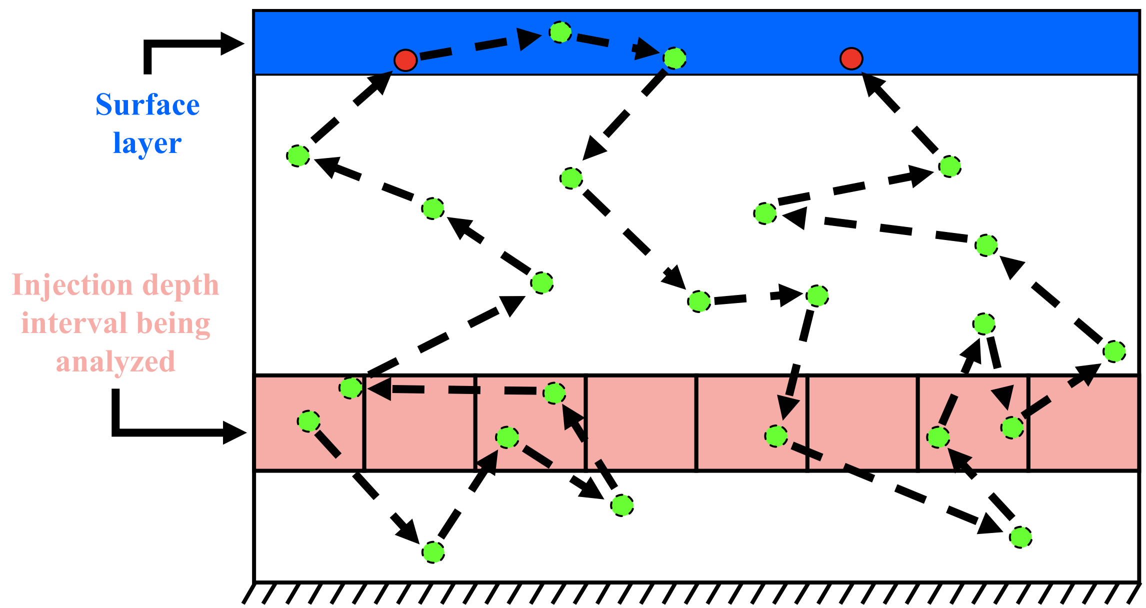
Efficiency

Introduction

One use of OGCMs is to evaluate the sequestration efficiency of injected carbon. Knowledge of the spatial distribution of sequestration efficiency can help in the quick identification of appropriate injection sites. In the OGCM framework, such a spatial distribution would be generated by running a separate simulation (or a separate tracer within the same simulation) for each grid cell evaluated. Characterizing the entire ocean domain in this manner would thus be extremely expensive, computationally. An adjoint sensitivity method for characterizing the sequestration efficiency of the entire domain of a global OGCM in a single simulation has recently been developed by Hill *et al*. (2003) and represents one way to ease the computational burden. Our Lagrangian random walk particle tracking model offers an alternate method to efficiently characterize the mean residence time (and hence sequestration efficiency) of an entire parent OGCM grid in one simulation. Since the model interface has been made as generic as possible, the Lagrangian model can be simulated with hydrodynamic output from many different OGCMs and thus serve as a useful intercomparison tool.

Simulating Mean Residence Time

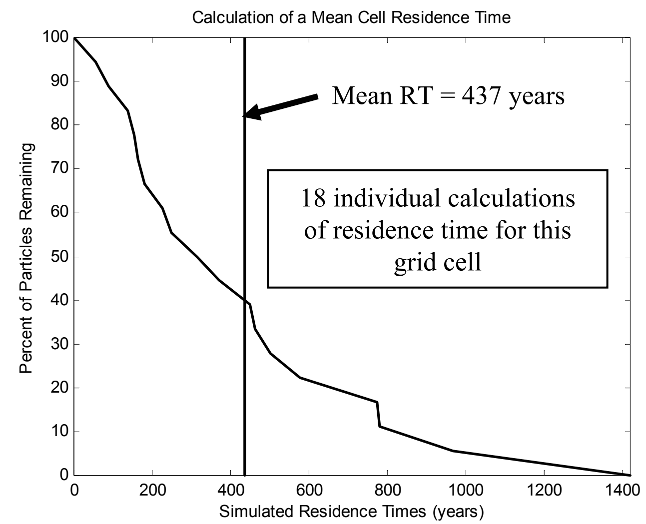
Rather than projecting particles onto the grid and continuing long-term calculations in Eulerian mode (as discussed in Application I), the particle-tracking model can be used for the entire simulation. This mode of operation is particularly efficient for studying sequestration efficiency since the mean residence time associated with each cell in the parent OGCM grid can be computed in a single simulation. Moreover, the calculation of mean residence time can be based not only on particles originating in a given cell, but also on particles that subsequently pass through that cell, as illustrated below.



When a particle first enters the surface layer (●), one can compute a residence time associated with all previously recorded locations (●) through which the particle has passed. Residence times for a given cell, which need not coincide with a parent OGCM grid cell, can be averaged.

A Preliminary Result

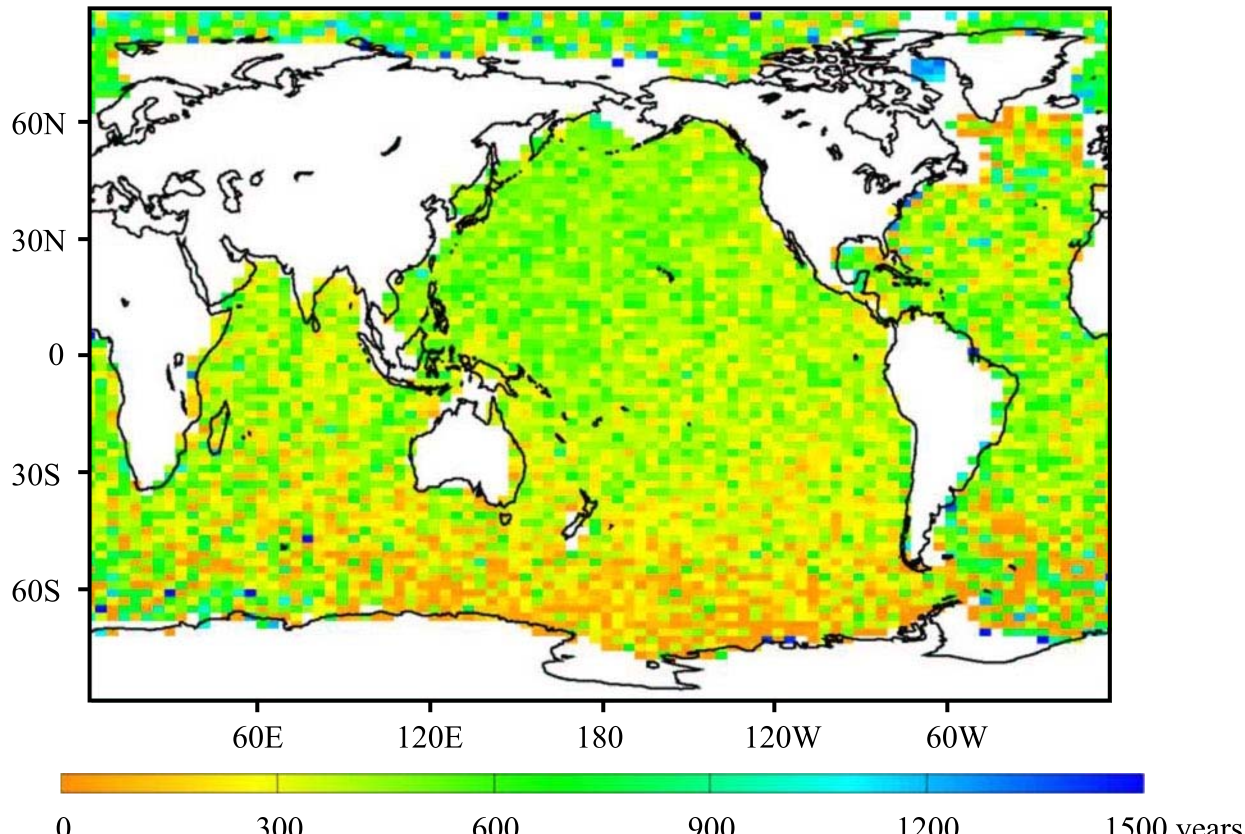
A preliminary simulation of this type has been carried out using the hydrodynamic information from the Lawrence Livermore National Laboratory (LLNL) OGCM, which has a horizontal resolution of 4º x 2º and 24 depth levels. The goal of the simulation was to characterize the mean residence time for the depth interval 1350 m to 1650 m (i.e., for an injection depth of about 1,500 m). About 8,200 particles were initially distributed across the ocean domain within this depth interval, and the simulation was run for 1,500 years. This resulted in about 410,000 individual estimates of residence time, which were binned into regions defined horizontally by the OGCM grid and vertically by the 1350 – 1650 m depth interval such that the spatial distribution of mean residence time could be calculated. The calculation is shown first for a single grid cell.



Distribution of predicted residence time estimates for particles originating in the region extending from 31 to 33ºN, 174 to 178ºW, and 1350 – 1650 m depth. The mean residence time for this region is calculated from these values.

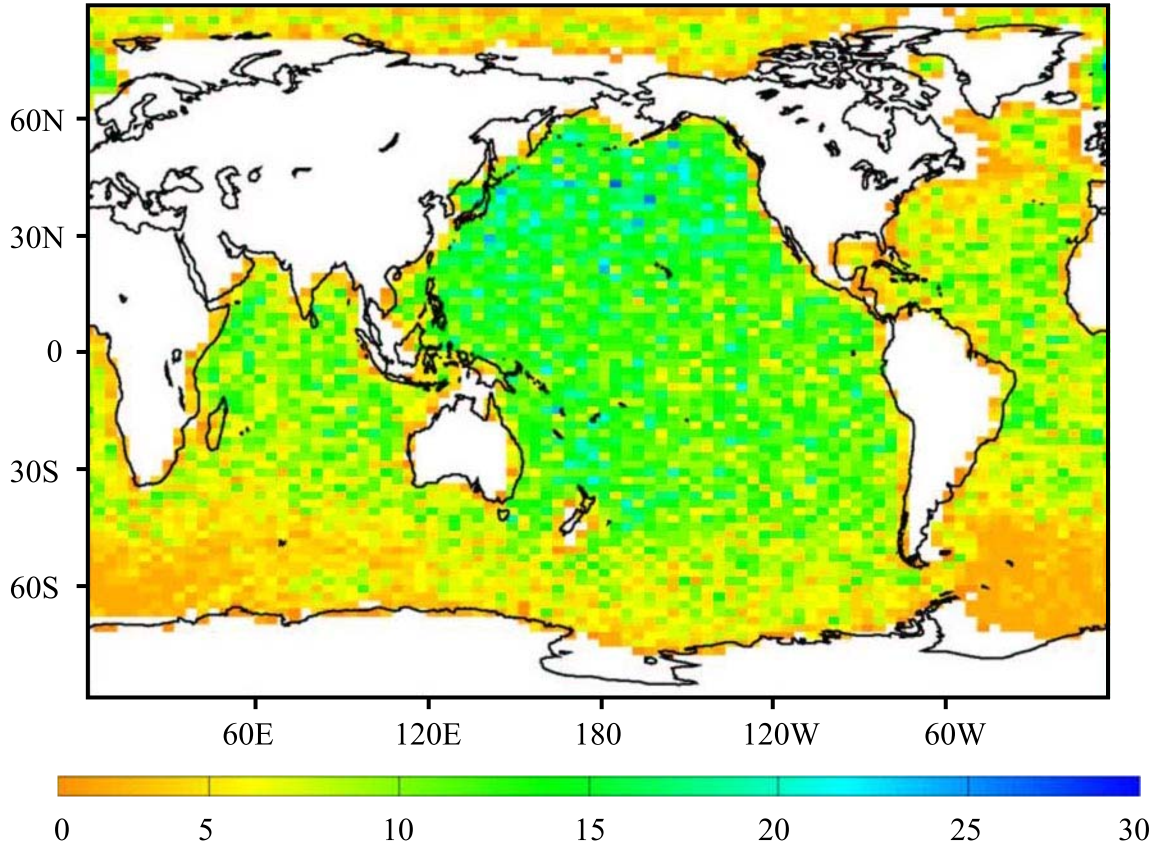
A Preliminary Result

The figure displays the spatial distribution of predicted mean residence times (in years) for a 1,500 year simulation using the LLNL OGCM hydrodynamic fields.



A Preliminary Result

The figure shows the spatial distribution of the number of data points upon which the preceding figure of mean residence times was based.



Ongoing and Future Work

- Model testing and application on intermediate and global scales is ongoing.
- Models are being enhanced with better numerical schemes and improved input/output; additional dynamics (e.g., air-water exchange) are being added.
- An interface between the Lagrangian models and near field models will be developed (emphasis will be placed on making this interface generic as well).
- The generic OGCM interface that has been developed will be tested by performing simulations with various configurations of MITgcm through increased collaboration with Prof. John Marshall and Dr. Mick Follows at the MIT Department of Earth and Planetary Sciences (EAPS).

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