Evaluation of the accuracy of an offline seasonally-varying matrix transport model for simulating ideal age

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Abstract

Newton-Krylov solvers for ocean tracers have the potential to greatly decrease the computational costs of spinning up deep-ocean tracers, which can take several thousand model years to reach equilibrium with surface processes. One version of the algorithm uses offline tracer transport matrices to simulate an annual cycle of tracer concentrations and applies Newton's method to find concentrations that are periodic in time. Here we present the impact of time-averaging the transport matrices on the equilibrium values of an ideal-age tracer. We compared annually-averaged, monthly-averaged, and 5-day-averaged transport matrices to an online simulation using the ocean component of the Community Earth System Model (CESM) with a nominal

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horizontal resolution of $1^\circ \times 1^\circ$ and 60 vertical levels. We found that increasing the time resolution of the offline transport model reduced a low age bias from 12% for the annually-averaged transport matrices, to 4% for the monthly-averaged transport matrices, and to less than 2% for the transport matrices constructed from 5-day averages. The largest differences were in areas with strong seasonal changes in the circulation, such as the Northern Indian Ocean. For many applications the relatively small bias obtained using the offline model makes the offline approach attractive because it uses significantly less computer resources and is simpler to set up and run.

Keywords: Implicit solver, ideal age, Newton-Krylov, offline, transport matrix, Global Ocean Modeling

1. Introduction

Tracers in the deep ocean take thousands of years to equilibrate with their sources and sinks (e.g. Primeau and Deleersnijder, 2009). As a result, ocean general circulation models that aim to simulate climatological tracers need long spin-up runs before reaching their equilibrium state. Even for models of moderate spatial resolution the computational burden is significant. The problem is further compounded by the CFL stability conditions, which impose ever smaller time-step size as resolution increases. Consequently, the push for models of ever increasing resolution means that the required computational resources will continue to outpace the expected increases in computational resources for the foreseeable future.

To avoid the excessive computational burden associated with the long time to tracer equilibrium, Li and Primeau (2008) and also Khatiwala (2008)

14 showed that a Newton-Krylov algorithm can be used to greatly decrease
 15 the computational time needed to spin up biogeochemical tracers to their
 16 seasonally-varying equilibrium state. The method solves for the periodic
 17 state of the annual cycle without solving for the transient spin-up of the
 18 tracers. This is accomplished by solving the coupled system of algebraic
 19 equations that propagate the tracer state of the ocean at the beginning of
 20 the year forward in time by exactly one year, such that the same tracer state is
 21 achieved at the end of the year. The algorithms proposed by Li and Primeau
 22 (2008) and also by Khatiwala (2008) used an offline tracer transport matrix
 23 with monthly temporal resolution to simulate the time-dependent seasonal
 24 cycle; however, the offline simulation is not an essential part of the algo-
 25 rithm. The Newton-Krylov algorithm can also be applied by using the full
 26 dynamical model to simulate the seasonal cycle needed to evaluate the trans-
 27 formation of the tracer (Lindsay, submitted). The tracer transport matrix
 28 is only indispensable for the construction of an effective preconditioner. In
 29 fact, using the online dynamical model to propagate the model tracer state
 30 forward for one year has the advantage of eliminating the errors incurred
 31 by approximating the continuous time-dependence of the advection-diffusion
 32 operator by a discrete set of 12 monthly transport operators. The main ad-
 33 vantages of the offline tracer transport matrix are that it uses significantly
 34 fewer computational resources and is in general much simpler to set up and
 35 run. Other useful additional capabilities are the ease of applying filtering
 36 operations to the transport matrix operators; the ease of using subsets of the
 37 operators (such as advection only); and the ability to restrict simulations to
 38 specific regions.

39 There is a substantial and growing body of work that is based on a
 40 transport matrix constructed by averaging the circulation of an OGCM (e.g.
 41 Primeau, 2005; Khatiwala et al., 2005; Kwon and Primeau, 2006; Kriest and
 42 Oschlies, 2011; Graven et al., 2012; Prieß et al., 2013; Bardin et al., 2014;
 43 Letscher et al., 2015), yet the error incurred by approximating the time-
 44 dependence of the circulation by step-wise constant tracer-transport matrices
 45 has never been rigorously assessed. The goal of this study is to start to fill
 46 in this gap by comparing an equilibrium tracer field obtained with an online
 47 simulation to one obtained from an offline matrix-transport model in which
 48 the seasonal cycle is represented by (i) an annually averaged matrix, (ii) a set
 49 of 12 monthly averaged matrices, and (iii) a set of 73 5-day averaged matri-
 50 ces. The tracer we consider is the ideal age (e.g. England, 1995; Deleersnijder
 51 et al., 2001; Primeau, 2005), because it nicely illustrates the long timescales
 52 of ocean transport and because it is straightforward to implement without
 53 any complicated tracer source-sink functions.

54 The main objective here is to quantify the difference the averaging of
 55 advection and diffusion fields that occurs in the offline approach makes on
 56 the computed ideal age, compared to using the online model with the full time
 57 resolution of the parent dynamic model. Are the differences using the offline
 58 approach sufficiently small that the precomputed transport matrices can be
 59 used for biogeochemical sensitivity studies, for calibrating sub-gridscale eddy
 60 diffusivity parameterization, or for the spin-up of biogeochemical tracers for
 61 the purpose of initializing transient simulations? We lay the groundwork by
 62 which to answer these questions quantitatively.

63 2. Methods

64 2.1. Ideal Age

65 The ideal age is defined as the mean time since a water parcel last had
 66 contact with the surface. It can be computed by solving the following initial
 67 value problem

$$\left\{ \begin{array}{l} \frac{\partial a}{\partial t} + \nabla \cdot [\mathbf{u} - \mathbf{K}\nabla] a = 1, \\ \hat{\mathbf{n}} \cdot \mathbf{K}\nabla a = 0, \text{ on all solid boundaries,} \\ a = 0 \text{ at the sea surface, } a(t_o) = a_o, \end{array} \right. \quad (1)$$

68 where a is the age, $\mathbf{u}$ is the fluid velocity, and $\mathbf{K}$ is the eddy diffusion tensor.
 69 The bold notation denotes vectors or tensors. “1” on the right hand side of
 70 the equation is an age source or rate of aging, i.e. 1 year per year.

71 We consider the case where the ocean circulation is perfectly periodic
 72 with a period of $\Delta T = 1$ year. This condition is satisfied provided the fluid
 73 velocity and eddy diffusivity tensor are both periodic with

$$\begin{aligned} \mathbf{u}(t + \Delta T) &= \mathbf{u}(t), \\ \mathbf{K}(t + \Delta T) &= \mathbf{K}(t). \end{aligned} \quad (2)$$

74 We are interested in the long-time asymptotic solution to equation (1) at
 75 which point the transients have died out so that the ideal age is also periodic
 76 with $a(t + \Delta T) = a(t)$.

77 2.2. The Dynamical Ocean Model

78 For this study we simulate the ocean circulation using the dynamical
 79 ocean model component (POP2) of the Community Earth System Model

80 (CESM), version 1.2 (Smith et al., 2010). The physical circulation was “spun-
 81 up” from rest for 250 years using the Common Ocean-ice Reference Experi-
 82 ments (CORE) climatological normal year forcing (Large and Yeager, 2004;
 83 Griffies et al., 2009; Large and Yeager, 2009), in which the same seasonal cycle
 84 is repeated every model year. The temperature and salinity were initialized
 85 from the January-mean climatology. Following the spin-up of the dynamics,
 86 the dynamical ocean model was run for an additional year during which all
 87 quantities needed to construct the model’s advection-diffusion transport op-
 88 erators in matrix form with monthly or 5-day time resolution were saved. The
 89 monthly-averaged or 5-day-averaged transport matrices provide representa-
 90 tions of the seasonal cycle. These transport matrices can also be averaged to
 91 produce the annually averaged transport matrix. Details of the construction
 92 of the offline transport matrices from the parent dynamical model are given
 93 in Bardin et al. (2014).

94 The length of the dynamical model spin-up was chosen based on the
 95 tradeoff between the use of computational resources and wall-clock time,
 96 and the model simulation time needed for the transients in the momentum
 97 equations to decay. The 250-year duration of the spin-up is inadequate for
 98 the transients in $\mathbf{u}$ and $\mathbf{K}$ to completely die out, but we nevertheless enforce
 99 the periodicity of the circulation when we solve equation (1). By doing so we
 100 suppress the effect of any intrinsic inter-annual variability on the ideal age.
 101 For the online model this is done by reinitializing the dynamical-model to the
 102 same model-year state conditions at the beginning of each year of iteration
 103 as described in Lindsay (submitted). For the offline model this is done by
 104 recycling the same transport matrices as described in Bardin et al. (2014).

Other details of the model configuration are as follows. The model has a dipolar grid with the convergence point normally found at the geographic North Pole displaced into Greenland; the transition from the grid following latitudinal and longitudinal lines starts at the Equator. The nominal $1^\circ \times 1^\circ$ horizontal grid has a higher meridional resolution of about 0.3° approaching the equator. In the vertical dimension there are 60 depth levels with vertical resolution of 10 m for the top 16 layers, increasing to 250 m near the bottom. The thickness of the top-most layer is allowed to vary from its 10 m thickness to include regional and temporal variations in sea surface height. Details of the numerical methods and discretization are given in the POP Reference Manual (Smith et al., 2010).

Transport of tracers in the model is achieved by a combination of explicitly resolved currents and parameterized sub-gridscale transport processes. Tracer transport is divided into an advection term, a “horizontal diffusion” term, and a “vertical diffusion” term. The advection term includes the explicitly resolved velocity as well as a bolus velocity that arises from the Gent McWilliams (GM) parameterization of mesoscale eddies (Gent and McWilliams, 1990). The advection term also incorporates a sill-overflow parameterization for the deep channel overflows in the Denmark Strait and the Faroe Banks Channel; and for continental shelf overflows in the Weddell and Ross Seas (Briegleb et al., 2010; Danabasoglu et al., 2010). A third-order upwind advection scheme is used to compute the advective tendencies of the explicitly-resolved and bolus velocities. The model also includes a purely diffusive parameterization of mixing by mesoscale eddies in the form of a diffusion tensor that is rotated so that the large “horizontal” diffusion acts along

130 isopycnal surfaces rather than across them (Redi, 1982). Thus the vertical
 131 diffusion term combines the vertical component of the along-isopycnal diffu-
 132 sion together with the diffusion from the K-profile parameterization (KPP)
 133 (Large et al., 1994), which accounts for the mixing induced by convective
 134 instabilities, shear instabilities, destabilizing tendencies associated with ver-
 135 tical gradients of salinity and temperature, as well as tidal mixing. The
 136 horizontal diffusion term captures the horizontal component of the along
 137 isopycnal diffusion.

138 *2.3. Newton Krylov Solver*

139 After being discretized in space the initial value problem (1) can be ex-
 140 pressed as a system of ordinary differential equations, which we denote sym-
 141 bolically as follows

$$\begin{cases} \frac{d}{dt}a(t) = \mathbf{f}(t, a(t)) \\ a(t_0) = a_0, \end{cases} \quad (3)$$

142 and whose solution can be expressed in terms of the following integral

$$a(t) = a(t_0) + \int_{t_0}^t \mathbf{f}(t', a(t'))dt'. \quad (4)$$

143 We define G as the integral over the time period

$$G(a(t_0)) \equiv \int_{t_0}^{t_0+\Delta T} \mathbf{f}(t', a(t'))dt', \quad (5)$$

144 such that the equilibrium condition, $a(t_0 + \Delta T) = a(t_0)$, is then given by

$$G(a(t_0)) = 0. \quad (6)$$

145 Further discretizing the time variable converts equation (6) into a system of
 146 algebraic equations, which can be solved using a Newton-Krylov method. We

147 note that evaluating G is equivalent to running the ideal age model forward
 148 in time for one year (ΔT) then subtracting the initial tracer state ($a(t_0)$)
 149 from the final tracer state ($a(t_0 + \Delta T)$).

150 We solve equation (6) using a Newton-Krylov algorithm in which we eval-
 151 uate $G(a(t_0))$ using the full online CESM-POP2 model (Lindsay, submitted)
 152 and using an offline model in which the advective-diffusive tracer flux di-
 153 vergence is computed using a discrete set of time-averaged tracer-transport
 154 matrices following Bardin et al. (2014).

155 Because the governing equation for the ideal age is linear, we can be
 156 assured that the solution is unique and that any difference we find between
 157 the online and offline solution can be attributed to the impact of using time-
 158 averaged transport matrices in the offline model.

159 *2.4. Online Evaluation of G*

160 The online evaluation of G consists of simulating the ideal age concur-
 161 rently with the dynamical simulation. The temporal resolution with which
 162 the circulation evolves and the time discretization used to evaluate the inte-
 163 gral defining G are therefore the same as that used to time-step CESM-POP2.
 164 As previously mentioned, the periodicity of the flow is enforced by initializing
 165 the dynamical model to the same initial state (that is, the same tempera-
 166 ture, salinity, velocity vectors, and sea-surface height) at the beginning of
 167 each one-year simulation (Lindsay, submitted). In CESM-POP2 the surface
 168 boundary condition for the ideal age tracer is implemented by resetting the
 169 ideal age to zero in the upper-most layer of the model at the end of every
 170 time-step.

171 2.5. Offline Evaluation of G

172 For the offline evaluation of G we use a discrete set of time-averaged
 173 transport matrices to compute the tracer flux divergence in the integrand
 174 of equation (5). Following Bardin et al. (2014), we separate the transport
 175 matrix into three terms

$$\mathbf{T} = \mathbf{A} + \mathbf{D} + \mathbf{H}, \quad (7)$$

176 where $\mathbf{A}$ includes the effect of advection and the tracer-transport effects of
 177 the sill overflow parameterization, $\mathbf{D}$ provides the effect of vertical diffusion,
 178 and $\mathbf{H}$ provides the effect of horizontal diffusion. These operators correspond
 179 to the POP Reference Manual (Smith et al., 2010) advection and diffusion
 180 operators $\mathbf{A} = -\mathcal{L}_T$, $\mathbf{D} = \mathcal{D}_V$, and $\mathbf{H} = \mathcal{D}_H$. The transport matrices are
 181 sparse and square, with dimensions given by the number of ocean grid-cells in
 182 the parent model. $\mathbf{A}$ and $\mathbf{H}$ are generated from the dynamical model using
 183 an Impulse-Response Function (IRF) while running the dynamical model
 184 through a one-year cycle. At the same time, the vertical diffusion coefficient
 185 is recorded; this allows $\mathbf{D}$ to be generated by explicit coding (Bardin et al.,
 186 2014).

187 We evaluate the integral in (5) by time-stepping the offline tracer-transport
 188 model through the seasonal cycle, using a set of piece-wise constant tracer-
 189 transport matrices. We consider three cases: a case with 73 5-day aver-
 190 aged matrices, a case with 12 monthly-averaged matrices, and a case with
 191 1 annually-averaged matrix; with each case having a set of the three com-
 192 ponent matrices in (7). Within each period (5 days, one month, or one
 193 year) the equation is stepped forward in time using an implicit first-order
 194 backward-Euler scheme for the vertical diffusion; 3rd-order Adams-Bashforth

195 for the advection; and first-order forward-Euler for horizontal diffusion and
 196 the age source-sink term. These schemes were chosen to accurately repre-
 197 sent the methods of tracer transport implemented in the online model. The
 198 surface boundary condition implementation in CESM-POP2 was used when
 199 time-stepping the tracer-transport model. When using direct matrix inver-
 200 sion techniques, the surface boundary condition was implemented with a
 201 first-order loss term with a loss frequency $1/\tau$ of $(1 \text{ hour})^{-1}$. This value is
 202 sufficiently high to effectively clamp the surface value of the ideal age to zero.

203 *2.6. Convergence of the Newton-Krylov Solver*

204 To ensure that any differences between the online and offline solutions are
 205 due to the approximation made by using piece-wise constant tracer transport
 206 matrices in the offline model we must ensure that equation (6) is solved with
 207 sufficient accuracy. The criterion that we employ is that the residual drift in
 208 the ideal age be less than 0.01 years per year for 99% of the ocean volume.
 209 This threshold is analogous to the threshold used for the OCMIP-2 $\Delta^{14}\text{C}$
 210 protocol (Lindsay, submitted).

211 Figure 1 shows a histogram of the remaining residuals after the conver-
 212 gence criterion is met for both the online and offline solutions. In a time-
 213 dependent simulation the remaining residual is expected to decay exponen-
 214 tially with time. Consequently, the contribution to the error in the ideal
 215 age from the residual drift is expected to be small; certainly much smaller
 216 than the differences between the online and offline solutions presented in the
 217 following section.

Figure 1: Histograms (a) and (b) show the distribution of the residual change over a one-year simulation of the equilibrium solution of ideal age, (a) for an online simulation, and (b) for a simulation run offline using monthly-averaged transport operators. Note that the x-axis is on a logarithmic scale. A typical criterion for acceptable convergence is that 99% of the volume has a residual of less than 10^{-2} years per year. The residual change is well below this criterion.

218 3. Comparison of Offline to Online Simulation Results

219 In this section the results of the online simulation are compared with
220 the results using annually-averaged, monthly-averaged, and 5-day-averaged
221 transport matrices. The purpose of this exercise is to determine how much
222 and where the biases are in the resulting equilibrium solution for ideal age,
223 compared to an equilibrium solution based on running the dynamic model
224 in an online simulation for the same year.

225 Figure 2 shows scatter-density diagrams comparing the ideal age equi-
226 librium solutions obtained using the annually-averaged, monthly-averaged,
227 and 5-day-averaged transport matrices to running online for the one-year
228 simulation.

229 The top panel compares the annually-averaged case to the online case.
230 The differences fall in a band below the one-to-one line on the scatter-density
231 diagram, indicating that ignoring the seasonal cycle results in a too-young
232 bias. On a volume-weighted basis, the ideal age computed using the annually-
233 averaged transport operator produces ages that are 12% younger than the
234 online simulation.

235 Using the monthly-averaged transport operator (middle panel) results in
236 a significantly smaller bias than the annually-averaged operator. The density
237 of points on the scatter density diagram is concentrated much more tightly
238 along the one-to-one line. The volume-weighted bias is now only -3.9%.

239 The bottom panel in Figure 2 compares the equilibrium solution for the 5-
240 day-averaged transport operator to the online case. The tracer-tracer scatter
241 density plot falls tightly on the one-to-one line with virtually no scatter. The
242 volume-weighted bias is only -1.6%.

Figure 2: Scatter density diagrams comparing the equilibrium solutions for ideal age using annually-averaged (top), monthly-averaged (middle), and 5-day-averaged (bottom), transport matrices versus using an online simulation. The “bias” is the average percent difference, on a volume weighted basis, when using the transport matrices rather than using an online simulation. The ideal age is younger using the transport matrices than when using the online simulation.

Figure 3: Depth profiles in meters of ideal age in years at selected locations in the Indian, Pacific, and Atlantic basins. The profiles compare the equilibrium solutions when the one-year simulation is run online versus using annually-averaged, monthly-averaged, and 5-day-averaged transport matrices offline. Only the profile using the annually-averaged transport matrices is clearly distinguishable from the online simulation. The topographical map shows the locations of the depth profiles.

243 The scatter-density diagrams provide information on how the ideal age
 244 computed in each of the cases differs with age. To examine how each case
 245 varies with depth, profiles of ideal age versus depth are provided. Figure 3
 246 shows depth profiles at locations throughout the ocean for the cases where
 247 the simulation used the transport matrices, and for the case where the on-
 248 line simulation was used. The accompanying topographical map shows the
 249 locations of the profiles. The right-hand column of profiles is in the Atlantic
 250 Basin, going from 50°N to 60°S traveling from top to bottom. The ideal age
 251 is nearly the same in all cases except for the profile in the Southern Ocean.

252 The Pacific basin, the middle column in Figure 3, shows a smaller but
 253 discernible difference for the annually-averaged transport matrix case, with
 254 the shapes of the profiles being similar. The largest differences are in the
 255 older waters, between 2000 and 4000 m. At 3000 m near the equator, the
 256 online simulation results in an ideal age of 2538 years. The difference with
 257 the annually-averaged case is 220 years; with the monthly-averaged case it is
 258 69 years; and with the 5-day-averaged case it is 29 years; indicating relative
 259 errors of 9%, 3%, and 1% respectively. If one considers a deep water parcel
 260 migrating slowly from the Southern Ocean northwards, and returning south-
 261 wards at depths of around 3000 m, that is consistent with the age profiles.
 262 It also is consistent with the absolute value of the bias becoming larger as
 263 the water increases in age; however, the relative (%) bias does not.

264 The Indian Basin, shown in the left-hand column, has the largest differ-
 265 ence between the annually-averaged transport matrices and all of the other
 266 cases. The northern Indian Ocean is an area of exceptionally strong seasonal
 267 variability. The largest differences are in the north end of the basin, in the

268 Arabian Sea (the 20°N panel); this is consistent with a comparison between
 269 the annually-averaged and monthly-averaged cases in Bardin et al. (2014).
 270 While the online simulation results in an ideal age of 1870 years at 20°N and
 271 2000 m depth, the annually-averaged case is 409 years younger, the monthly-
 272 averaged case is 59 years younger, and the 5-day-averaged case is 20 years
 273 younger, corresponding to relative errors of 22%, 3%, and 1% respectively.
 274 Near the equator at 2000 m depth, the online simulation results in an ideal
 275 age of 1705 years. The annually-averaged case is 297 years younger; the
 276 monthly-averaged case is 66 years younger; and the 5-day-averaged case is
 277 19 years younger; indicating relative errors of 17%, 4%, and 1% respectively.

278 The three profiles in the Southern Ocean at 60°S are remarkably similar,
 279 within a few years of each other at the same depth. At 2000 m, the online
 280 simulation results in an ideal age of around 750 years; the difference for the
 281 annually-averaged case is 101 years; the monthly-averaged case is 28 years
 282 younger; and the 5-day-averaged case 13 years younger; indicating relative
 283 errors of 13%, 4%, and 2% respectively.

284 In Figures 4, 5, 6, and 7 we show the relative error for the ideal age
 285 computation based on the annually-averaged, monthly-averaged, and 5-day
 286 averaged transport operator at 400 m, 1000 m, 3000 m, and 4000 m depths.
 287 For all cases the relative error decreases with increasing temporal resolution
 288 of the transport matrices.

289 At 400 m (Figure 4), a band near the equator as well as the Southern and
 290 South-Eastern coast of Australia show older ideal ages for the offline model,
 291 while the rest of the ocean, and especially the high-latitude North Atlantic
 292 Ocean and Eastern Mediterranean basin show a youthful bias.

Figure 4: At a depth of 400 m, the top panel shows the equilibrium ideal age using the online simulation. The bottom three panels show the percent difference when the simulation is run using the annually-averaged, monthly-averaged, and 5-day averaged transport matrices. A positive percent difference means the offline model has older ideal age than the online model.

Figure 5: At a depth of 1000 m, the top panel shows the equilibrium ideal age using the online simulation. The bottom three panels show the percent difference when the simulation is run using the annually-averaged, monthly-averaged, and 5-day averaged transport matrices. A positive percent difference means the offline model has older ideal age than the online model.

Figure 6: At a depth of 3000 m, the top panel shows the equilibrium ideal age using the online simulation. The bottom three panels show the percent difference when the simulation is run using the annually-averaged, monthly-averaged, and 5-day averaged transport matrices. A positive percent difference means the offline model has older ideal age than the online model.

Figure 7: At a depth of 4000 m, the top panel shows the equilibrium ideal age using the online simulation. The bottom three panels show the percent difference when the simulation is run using the annually-averaged, monthly-averaged, and 5-day averaged transport matrices. A positive percent difference means the offline model has older ideal age than the online model.

293 At 1000 m (Figure 5), the relative differences with the online simulation
294 are less than for the 400 m case. The Labrador Sea and the Mediterranean
295 are still showing a substantial youthful bias. For the annually-averaged case,
296 the percent differences in the North Pacific, where some of the oldest waters
297 reside, are significantly less than the 400 m case.

298 At 3000 m (Figure 6), the age bias along the equator that was evident
299 higher up in the water column disappears. The relative error field shows a
300 youthful bias at high latitudes where deep waters are newly formed. In gen-
301 eral this relative error decreases as water moves away from the high latitude
302 formation regions, indicating that there is little accumulation of transport
303 errors along the flow. A notable exception is the north-eastern Indian Ocean
304 basin where masses have a local relative error maximum for the annually-
305 averaged operator and for the monthly-averaged operators.

306 The ages at 4000 m (Figure 7), reflect the pattern seen at 3000 m. The
307 differences of the monthly-averaged case and the 5-day averaged case with
308 the online simulation are relatively small.

309 4. Discussion

310 The general agreement between the online equilibrium solution and the
311 solutions using the offline transport matrices gives confidence that the offline
312 simulated equilibrium solution is representative of the online model behavior.
313 For applications where the interest is in the ventilation of the deep ocean,
314 even the annually-averaged transport operator captures the first order ven-
315 tilation patterns of the parent model. For applications where relative errors
316 of up to 10% are tolerable, the monthly averaged operators appear adequate

317 for waters below 1000 m; the 5-day averaged operators have relative errors
318 that are generally less than 10% for depths extending up to 400 m below the
319 surface. We note these errors are small compared to the errors of the online
320 model in relation to observationally based ideal age estimates, which are on
321 the order of 100% in the deep North Pacific basin, i.e. ~ 2800 years for
322 CESM-POP2 versus ~ 1400 years for the observationally constrained model
323 of DeVries and Primeau (2011).

324 For the upper-most ocean, the ideal age is not the best tracer with which
325 to evaluate the offline tracer transport matrix. Because the ideal age is
326 identically zero at the surface, it is not a good tracer to capture the strong
327 seasonality of the circulation in the surface layers. Other tracers that have
328 more realistic boundary conditions at the surface would provide a better
329 means of evaluating the temporal resolution of the tracer transport matrices
330 in the upper-most ocean.

331 Given that the offline matrix approach results in some bias with respect
332 to the online model (unless the transport matrices are saved for every time-
333 step of the parent model), one might wonder what the advantages of using
334 the offline approach are that make it compelling. The main reasons are the
335 ease with which new tracers can be implemented in the offline model and the
336 substantial savings in computer resources; these lead to a much shorter real
337 time to generate a close approximation. The savings in computer resources
338 can be illustrated by those used in the one-year simulation: for similar wall-
339 clock times, the online simulation uses 16 computer nodes, compared to 1
340 computer node when using the monthly-averaged transport matrices. In
341 the offline model, tracer source-sink functions can be easily coded in a high

level language like Matlab without much of a performance penalty because most of the heavy computational lifting consists of matrix-vector products and the solution of a tri-diagonal system of linear equations. While these heavy computational operations can easily be implemented in Matlab with a single line of code, we have found it beneficial to implement them in C++ to reduce the computational time; however, a modeler need not be aware of these details to implement new tracer source-sink functions in the offline model. Appendix A provides software design details. Appendix B provides more computer resource details and a table of comparisons for the online and various offline simulations.

5. Conclusions

We have used the implicit Newton-Krylov method to obtain the equilibrium solution for ideal age using the offline annually-averaged, monthly-averaged, and 5-day-averaged transport matrices, and using the online dynamic model itself. This has shown that compared to using the online dynamic model, a volume-weighted bias of 12% younger results when annually-averaged transport matrices are used, but only 3.9% younger when monthly-averaged transport matrices were used, and 1.6% younger when 5-day averaged transport matrices were used. That these errors decrease as the temporal resolution of the transport matrix operator increases confirms that the transport matrices faithfully capture the circulation of the parent model. Furthermore, the relative errors incurred when computing the ventilation ages of the deep ocean using monthly-averaged transport matrices are small relative to the age biases of the online model in relation to the observations.

366 This makes the offline transport matrix model a reasonably accurate method
367 that is easy-to-use and computationally efficient for simulating tracer distri-
368 butions in equilibrium with their source-sink functions.

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384 **Appendix A. Computation Details**

385 C++ coding was used to enhance the performance of the matrix-vector
386 products and the solution of the tri-diagonal system of linear equations.
387 These occur during the one-year simulation, which uses the bulk of the com-
388 puter time. The C++ Matlab “mex” interface function implements three

OpenMP-multithreaded computational kernels: the matrix-vector product, the tri-diagonal matrix factorization, and the subsequent linear equation solution. The tri-diagonal matrix routines exploit the property that the vertical diffusion operation is decoupled by physical water column. Hence each thread can factor the part of a matrix associated with just one water column, and similarly can solve just the associated part of the linear equation. Each such block is factored using Lapack’s “dgttrf” function, and the solver uses the “dgttrs” function (Anderson et al., 1999).

Appendix B. Computer Resources

A comparison of the computer resources and wall-clock time for running one-year tracer simulations using the online and offline model is summarized in Table B.1. On the order of 20-30 one-year simulations are needed for the Newton-Krylov solver to converge. The comparisons are from runs accomplished at the NCAR Yellowstone facility. There are several types of processors at the facility. The “Yellowstone” processors are 2.6-GHz Intel Xeon ES-2670 processors; each “Yellowstone” node has 16 of these processors, and 32 GB of memory. “Geyser” processors are 2.4-GHz Intel Xeon E7-4870 processors; each “Geyser” node has 40 processors and 1 TB of memory.

The table also shows the computational time for obtaining the equilibrium ideal age for the annually averaged flow by direct matrix inversion using the MUMPS solver (Amestoy et al., 2001). This is feasible because the annually-averaged transport matrix is a steady-state transport operator. A direct solution is provided for $\mathbf{T}a = S$, where S is a constant source-sink term. The total wall-clock time for the direct solution of the steady-state

transport model is significantly less than when Newton-Krylov is used (30 minutes versus 9 hours); but the memory requirement is much larger (300 GB versus 112 GB using Newton-Krylov on a time-stepping simulation with an in-memory factored preconditioner, or 6 GB for the time-stepping simulation only). The direct solution is most efficiently executed on the “Geyser” configuration because of the large memory availability.

Simulation Type	Nodes	Wall-Clock Time
online	16 Yellowstone	27 min. per model year
annually-averaged	1 Yellowstone	19 min. per model year
monthly-averaged	1 Yellowstone	19 min. per model year
5-day-averaged	1 Yellowstone	49 min. per model year
annually-averaged (MUMPS)	1 Geyser	30 min. equilibrium solution

Table B.1: Wall-clock time and number of computer nodes used for online and offline one-year simulations at the NCAR Yellowstone facility. Each Yellowstone node has 16 processors and 32 GB of memory; each Geyser node has 40 processors and 1 TB of memory. Each Newton-Krylov solution takes 20 - 30 one-year simulations to converge to the equilibrium solution. MUMPS uses a direct matrix inversion to compute the equilibrium solution.

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