A Newton-Krylov Solver for Fast Spin-up of Online Ocean Tracers

Keith Lindsay

*National Center for Atmospheric Research, P.O. Box 3000, Boulder, CO 80307-3000,
USA*

Abstract

We present a Newton-Krylov based solver to efficiently spin up tracers in an online ocean model. We demonstrate that the solver converges, that tracer simulations initialized with the solution from the solver have small drift, and that the solver takes orders of magnitude less computational time than the brute force spin-up approach. To demonstrate the application of the solver, we use it to efficiently spin up the tracer ideal age with respect to the circulation from different time intervals in a long physics run. We then evaluate how the spun-up ideal age tracer depends on the duration of the physics run, i.e., on how equilibrated the circulation is.

Keywords: Newton-Krylov, Tracers, Ideal Age, Ocean Modelling

1. Introduction

Analysis of ocean tracer simulations is complicated by the presence of drift (i.e., the simulated ocean tracers are not in balance with their boundary conditions and the ocean circulation). Drift in simulated tracers adds

Email address: `klindsay@ucar.edu` (Keith Lindsay)

Preprint submitted to Ocean Modelling

November 1, 2016

5 uncertainty to comparisons with observations and complicates the interpretation of tracer processes (e.g., source-sink terms and couplings between
 6 tracers), particularly when these processes are non-linear. Tracer drift also
 7 complicates the evaluation of tracer’s response to transient forcing (e.g., rising atmospheric CO₂ or anthropogenic nutrient inputs), because the tracer’s
 8 response can depend on the state of the tracer itself. Therefore, the capacity to generate tracer distributions in balance with their boundary conditions and the ocean circulation is advantageous. Because ventilation of
 9 the deep ocean takes in excess of 1000 years (Holzer and Primeau, 2010; DeVries and Primeau, 2011; Khatiwala et al., 2012), brute force tracer spin-up, running the tracers forward in time until this balance is reached, takes
 10 thousands of simulated years (i.e., multiple ventilation timescales). Running
 11 ocean models at a resolution typical of contemporary climate models (about
 12 1° or $\mathcal{O}(10^6)$ grid points) for this duration is computationally expensive, and
 13 often prohibitive.

20 Previous efforts have overcome this hurdle, in the context of offline tracer transport, by using Newton-Krylov based solvers to directly solve for the
 21 spun-up tracer distributions (Li and Primeau, 2008; Khatiwala, 2008; Bardin et al.,
 22 2014). One approach to spin up tracers for use in an online ocean model is
 23 to use a Newton-Krylov solver in conjunction with an offline tracer transport model, where the offline model is using the circulation of the online
 24 model. A disadvantage of this approach is that offline models typically use
 25 approximations in their representation of the online model’s circulation (e.g.,
 26 using temporally averaged circulation operators), and it is unclear how these
 27 approximations affect the spun-up tracer distributions. While Bardin et al.

30 (2016) shows that the impact of these approximations on spun-up ideal age is
 31 small if the circulation is sampled frequently enough, the significance of the
 32 impact likely depends on the timescales of the processes affecting the tracers
 33 being spun up. Another disadvantage of this approach is that in practice,
 34 the tracers are either implemented separately in both the offline and online
 35 models, or the tracers are implemented in a way that is compatible with
 36 both models. For complex tracers, such as ecosystem models, the burden
 37 of having multiple tracer implementations, or of implementing the tracers
 38 compatibly with both models, can be excessive. Furthermore, it would not
 39 be easy to extend this approach to spinning up the active tracers of an ocean
 40 model. Because of these disadvantages, it is desirable to have a fast spin-up
 41 technique that is directly applicable to online ocean tracer simulations.

42 We present here the successful application of a Newton-Krylov based
 43 solver to efficiently spin up passive tracers in online ocean tracer simula-
 44 tions. We demonstrate this tool by efficiently spinning up the tracer ideal
 45 age (Thiele and Sarmiento, 1990) with respect to the circulation from dif-
 46 ferent time intervals in a long physics run. We further evaluate how the
 47 spun-up ideal age tracer depends on the duration of the physics run, i.e., on
 48 how equilibrated the circulation is.

49 We describe, in Section 2, our formulation of the spin-up problem and
 50 the Newton-Krylov solver that we have developed to solve it, deferring some
 51 of the technical implementation details into appendices. We also describe in
 52 that section the computational experiments in which we use the solver. We
 53 present the results of these experiments in Section 3, discuss these results in
 54 Section 4, and give some concluding remarks in Section 5.

55 2. Methods

56 We first state the definition that we use of the spin-up problem for generic
 57 ocean tracers, mostly following the notation of Khatiwala (2008). Tracer
 58 concentrations, denoted by $\mathbf{c}(t)$, evolve in time according to the equation

$$\frac{d\mathbf{c}}{dt} = \mathbf{f}(t, \mathbf{c}), \quad (1)$$

59 where $\mathbf{f}$ denotes the sum of mixing, advective, and source-sink tendencies of
 60 the tracers. In practice, $\mathbf{c}$ is a vector whose component values correspond
 61 to the ocean model’s spatial discretization of tracers (e.g., grid cell means
 62 or spectral element decomposition coefficients). We use bold to denote vec-
 63 tors, such as $\mathbf{c}$, matrices, and other vector-valued operators. The solution
 64 of Eq. (1), with tracer concentrations at time t_0 specified by $\mathbf{c}(t_0)$, can be
 65 written as

$$\mathbf{c}(t) = \mathbf{\Phi}(t, t_0, \mathbf{c}(t_0)). \quad (2)$$

66 The spin-up problem is that for a given t_0 and time duration Δt , we seek
 67 initial tracer concentrations $\mathbf{c}(t_0)$ that leads to $\mathbf{c}(t_0 + \Delta t) = \mathbf{c}(t_0)$. That is,
 68 we seek a solution $\mathbf{c}(t_0)$ of the equation

$$\mathbf{G}(\mathbf{c}(t_0)) \equiv \mathbf{\Phi}(t_0 + \Delta t, t_0, \mathbf{c}(t_0)) - \mathbf{c}(t_0) = \mathbf{0}. \quad (3)$$

69 Such a solution is said to be spun-up with respect to the ocean model’s circu-
 70 lation over the time interval t_0 to $t_0 + \Delta t$. Δt is typically an integer number
 71 of years. We refer the reader to Section 4.1 for some practical implications
 72 of this formal definition of the tracer spin-up problem.

73 The brute force approach to generating a spun-up solution to Eq. (3) is
 74 to run the tracers forward in time repeatedly from t_0 to $t_0 + \Delta t$, initializing

75 the tracer concentrations at t_0 from the previous values at $t_0 + \Delta t$. Mathe-
 76 matically, this is equivalent to using fixed-point iterations on Eq. (2) to solve
 77 Eq. (3),

$$\mathbf{c}_{n+1} = \Phi(t_0 + \Delta t, t_0, \mathbf{c}_n). \quad (4)$$

78 We note that repeatedly performing fixed-point iterations is equivalent to
 79 running the tracers forward in time from t_0 to $t = \infty$, if one repeats periodi-
 80 cally the model's circulation and physical state variables forward in time from
 81 the interval t_0 to $t_0 + \Delta t$. As stated in Section 1, it takes thousands of model
 82 years to spin up tracers with such an approach, which is computationally
 83 expensive.

84 A different approach to find spun-up tracer concentrations is to apply
 85 Newton's method to Eq. (3). Newton's method is an iterative method to
 86 approximate the solution of a system of equations that proceeds as follows.
 87 Given the current iterate, $\mathbf{c}_n$, $\mathbf{G}(\mathbf{c})$ is approximated with a linearization in
 88 the neighborhood of $\mathbf{c}_n$,

$$\mathbf{G}(\mathbf{c}_n + \delta \mathbf{c}_n) \approx \mathbf{G}(\mathbf{c}_n) + \mathbf{J}_n \delta \mathbf{c}_n, \quad (5)$$

89 $\delta \mathbf{c}_n$ is found such that the right-hand side of Eq. (5) is zero,

$$\mathbf{J}_n \delta \mathbf{c}_n = -\mathbf{G}(\mathbf{c}_n), \quad (6)$$

90 and the next Newton iterate is set to

$$\mathbf{c}_{n+1} = \mathbf{c}_n + \delta \mathbf{c}_n. \quad (7)$$

91 In these equations, $\mathbf{J}_n$ is the Jacobian of $\mathbf{G}$ evaluated at $\mathbf{c}_n$,

$$\mathbf{J}_n \equiv \left. \frac{\partial \mathbf{G}}{\partial \mathbf{c}} \right|_{\mathbf{c}_n}. \quad (8)$$

92 It represents how increments, $\delta \mathbf{c}$, to the tracer concentrations, $\mathbf{c}$, lead to
 93 changes in $\mathbf{G}$, as they evolve over the time interval t_0 to $t_0 + \Delta t$. Because
 94 the duration of the interval, Δt , spans many model time steps (i.e., we are
 95 not considering instantaneous changes), $\mathbf{J}_n$ is not sparse, making it difficult
 96 to compute all of its entries. This precludes using a direct method to solve
 97 Eq. (6). We instead use an iterative method.

98 Krylov subspace methods (Saad, 2003) are a class of iterative methods
 99 for solving $\mathbf{Ax} = \mathbf{b}$ that work by minimizing the residual $\mathbf{r} = \mathbf{b} - \mathbf{Ax}$ over
 100 vectors from a Krylov subspace

$$\mathcal{K}_m(\mathbf{A}, \mathbf{b}) = \text{span} \{ \mathbf{b}, \mathbf{Ab}, \mathbf{A}^2\mathbf{b}, \dots, \mathbf{A}^{m-1}\mathbf{b} \}. \quad (9)$$

101 A notable feature of these methods is that they only utilize the matrix $\mathbf{A}$
 102 through matrix-vector multiplications with $\mathbf{A}$, they do not directly access
 103 the individual entries of $\mathbf{A}$. Because of this feature, they are well suited for
 104 solving $\mathbf{Ax} = \mathbf{b}$ when the entries of $\mathbf{A}$ are not available, provided that one
 105 can compute matrix-vector multiplications with $\mathbf{A}$. Matrix-vector multipli-
 106 cations with our Jacobian matrix $\mathbf{J}_n$ can be approximated with the finite
 107 difference approximation

$$\mathbf{J}_n \delta \mathbf{c} \approx (\mathbf{G}(\mathbf{c}_n + \sigma \delta \mathbf{c}) - \mathbf{G}(\mathbf{c}_n)) / \sigma, \quad (10)$$

108 for a suitably chosen scalar σ . For our $\mathbf{G}$, the right-hand side of Eq. (10)
 109 can be evaluated with two model runs, one to evaluate each $\mathbf{G}$ term, or a
 110 single model run if $\mathbf{G}(\mathbf{c}_n)$ has been previously computed. Krylov subspace
 111 methods are thus a feasible way to solve Eq. (6). The particular Krylov
 112 subspace method that we use is GMRES (Saad and Schultz, 1986), following
 113 the presentation in Saad (2003).

114 Summarizing, we use Newton’s method, Eqs. (6) and (7), to solve Eq. (3).
 115 The increment in Newton’s method, $\delta \mathbf{c}_n$, is obtained by using GMRES to
 116 solve Eq. (6). The matrix-vector multiplications required by GMRES are
 117 evaluated using Eq. (10). There are a number of technical details involved in
 118 implementing this Newton-Krylov solver. In particular, the batch computing
 119 environment that our ocean model is run within leads to some complications.
 120 We refer the reader to Appendix A for these technical details.

121 2.1. Krylov Preconditioner

122 Following Li and Primeau (2008) and Khatiwala (2008), we apply a pre-
 123 conditioner to Eq. (6) to improve the convergence rate of the Krylov solver.
 124 We use a left preconditioner, yielding

$$\mathbf{P}_n \mathbf{J}_n \delta \mathbf{c}_n = -\mathbf{P}_n \mathbf{G}(\mathbf{c}_n), \quad (11)$$

125 where $\mathbf{P}_n$ is the preconditioner matrix. In order to improve the convergence
 126 rate of the Krylov solver, $\mathbf{P}_n$ should approximate the inverse of $\mathbf{J}_n$. With the
 127 introduction of a left preconditioner into the Krylov solver, matrix operations
 128 using the matrix $\mathbf{J}_n$, such as matrix-vector multiplications, are replaced with
 129 matrix operations using the matrix $\mathbf{P}_n \mathbf{J}_n$. These latter matrix-vector multi-
 130 plications are implemented by first evaluating a matrix-vector multiplication
 131 using $\mathbf{J}_n$, evaluated using Eq. (10), and then multiplying the result by $\mathbf{P}_n$.
 132 In order to be of practical benefit, computing matrix-vector multiplications
 133 with $\mathbf{P}_n$ needs to be computationally feasible.

134 We use the same type of conditioner that Li and Primeau (2008) and
 135 Khatiwala (2008) both use. Following the derivation in Khatiwala (2008),
 136 we construct $\mathbf{P}_n$ by introducing $\tilde{\Phi}$, an approximation to the ocean model’s

137 evaluation of Φ , and set P_n to be inverse of $\tilde{J}$, the Jacobian that corresponds
 138 to $\tilde{\Phi}$. As shown by Khatiwala (2008), a choice for $\tilde{\Phi}$ that works well is to
 139 replace the ocean model's time stepping with a single backward Euler time
 140 step over the time interval t_0 to $t_0 + \Delta t$,

$$\tilde{\Phi}_K - \mathbf{c}(t_0) = \Delta t \mathbf{f}(t_0 + \Delta t, \tilde{\Phi}_K), \quad (12)$$

141 where the K subscript denotes that this is the approximation of Khatiwala
 142 (2008). In order to better capture the mean of the ocean model's circulation,
 143 we replace the instantaneous mixing and advective operators that effectively
 144 appear on the right-hand side of Eq. (12) with their time-average over the
 145 time interval t_0 to $t_0 + \Delta t$, yielding

$$\tilde{\Phi} - \mathbf{c}(t_0) = \Delta t \overline{\mathbf{f}}(\tilde{\Phi}), \quad (13)$$

146 where the overbar represents time-averaging. Note that while the operators
 147 of $\overline{\mathbf{f}}$ are time-averaged, they are being applied in Eq. (13) to instantaneous
 148 values of $\tilde{\Phi}$. One can derive, see Appendix B, that the inverse of $\tilde{J}$ for this
 149 $\tilde{\Phi}$ is

$$P_n = \tilde{J}^{-1} = \left(\Delta t \frac{\partial \overline{\mathbf{f}}}{\partial \mathbf{c}} \right)^{-1} - \mathbf{I}, \quad (14)$$

150 where $\mathbf{I}$ is the identity matrix. It then follows that the matrix-vector product
 151 $P_n \mathbf{v}$, for an arbitrary vector $\mathbf{v}$, is

$$P_n \mathbf{v} = \left(\Delta t \frac{\partial \overline{\mathbf{f}}}{\partial \mathbf{c}} \right)^{-1} \mathbf{v} - \mathbf{v}. \quad (15)$$

152 Computing this requires solving

$$\left(\Delta t \frac{\partial \overline{\mathbf{f}}}{\partial \mathbf{c}} \right) \mathbf{x} = \mathbf{v} \quad (16)$$

153 for $\mathbf{x}$. The matrix that appears in this system of linear equations, $\Delta t \partial \bar{\mathbf{f}} / \partial \mathbf{c}$,
 154 represents how instantaneous tracer tendencies from the time-averaged op-
 155 erators of $\bar{\mathbf{f}}$ depend on tracer concentrations. These partial derivatives, of
 156 $\bar{\mathbf{f}}$ with respect to $\mathbf{c}$, are localized in space, because they are of instanta-
 157 neous, not time-integrated, quantities. This localization in turn leads to
 158 $\Delta t \partial \bar{\mathbf{f}} / \partial \mathbf{c}$ being sparse. Systems of linear equations with sparse matrices,
 159 such as this, can be solved with existing sparse matrix libraries, such as
 160 SuperLU (Li et al., 1999; Li and Demmel, 2003). Because some aspects of
 161 the construction of this matrix are specific to our ocean model, we defer a
 162 description of the construction of this matrix to Section 2.3, after we have
 163 described our ocean model.

164 *2.2. Ocean Model Description*

165 We have implemented the Newton-Krylov solver described above in the
 166 ocean component (Danabasoglu et al., 2012) of version 1 of the Community
 167 Earth System Model (CESM1) (Hurrell et al., 2013), which is based on
 168 version 2 of the Parallel Ocean Program (POP2) (Smith et al., 2010). In our
 169 numerical experiments, POP2 uses a nominal 1° curvilinear grid, with 320
 170 grid cells in the zonal direction and 384 grid cells in the meridional direction.
 171 The vertical grid has 60 layers. At this spatial resolution, a parameterization
 172 of the effects of mesoscale eddies is necessary, and POP2 includes the Gent-
 173 McWilliams isopycnal mixing scheme (Gent and McWilliams, 1990). As de-
 174 scribed in Danabasoglu et al. (2012), some of the other parameterizations of
 175 POP2 include the KPP vertical mixing scheme (Large et al., 1994) and a
 176 parameterization of overflows (Danabasoglu et al., 2010). Our experiments
 177 use an active sea ice model, the sea ice component of CESM1 (Holland et al.,

2012), which is based on version 4 of the Los Alamos Sea Ice Model (CICE4)
 (Hunke and Lipscomb, 2008). The sea ice model uses the same horizontal
 grid as the ocean model. The surface forcing in our experiments is the nor-
 mal year (NY) forcing of Large and Yeager (2004).

2.3. Applying the Krylov Preconditioner

As stated in Section 2.1, computing the matrix-vector product $\mathbf{P}_n \mathbf{v}$ in-
 volves solving the system of linear equations in Eq. (16) and applying Eq. (15).
 So it is necessary to construct the matrix $\Delta t \partial \bar{\mathbf{f}} / \partial \mathbf{c}$, subsequently denoted
 by $\mathbf{Q}$, and solve the corresponding system of linear equations. The entries
 of the matrix $\mathbf{Q}$ are the partial derivatives of the tracer tendencies from the
 time-averaged mixing, advective, and source-sink operators with respect to
 the tracer concentrations.

Motivated by the transport matrix method of Khatiwala et al. (2005),
 computation of the partial derivatives of tendencies from time-averaged linear
 operators (e.g., lateral mixing and advection) can be done as follows. We
 write tracer concentrations as a weighted sum of Kronecker delta functions

$$\mathbf{c} = \sum_i c^i \boldsymbol{\delta}^i, \quad (17)$$

where i is a grid cell index, c^i is the value of $\mathbf{c}$ at grid cell i , and $\boldsymbol{\delta}^i$ is a
 Kronecker delta function at grid cell i (i.e., $\boldsymbol{\delta}^i$ is one at grid cell i and zero
 at other grid cells). Denoting the linear operator by $\mathcal{L}$, and its time-average
 by $\bar{\mathcal{L}}$, we have

$$\bar{\mathcal{L}}(\mathbf{c}) = \bar{\mathcal{L}}\left(\sum_i c^i \boldsymbol{\delta}^i\right) = \sum_i c^i \bar{\mathcal{L}}(\boldsymbol{\delta}^i), \quad (18)$$

198 where we have used the linearity of $\overline{\mathcal{L}}$. The derivative of $\overline{\mathcal{L}}(\mathbf{c})$ with respect
 199 to c^j is thus

$$\frac{\partial \overline{\mathcal{L}}(\mathbf{c})}{\partial c^j} = \sum_i \frac{\partial c^i}{\partial c^j} \overline{\mathcal{L}}(\boldsymbol{\delta}^i) = \overline{\mathcal{L}}(\boldsymbol{\delta}^j) = \overline{\mathcal{L}(\boldsymbol{\delta}^j)}, \quad (19)$$

200 where the final equality holds because $\boldsymbol{\delta}^j$ is independent of t . This shows that
 201 the partial derivatives of the tendencies from $\overline{\mathcal{L}}$ are equal to the time-averaged
 202 tendencies of $\mathcal{L}$ applied to Kronecker delta functions.

203 We compute these terms with the aid of impulse response (IR) tracers,
 204 which are tracers that are reset every time step to Kronecker delta functions
 205 (i.e., impulses). The desired partial derivatives are the time-average of the
 206 result of applying $\mathcal{L}$ to these IR tracers, which can be included in the ocean
 207 model's diagnostic output. A naïve implementation of the IR tracers would
 208 have one tracer per grid cell. This would lead to $\mathcal{O}(10^6)$ tracers for our
 209 model grid, which is not practical to run with. However, for operators that
 210 are localized in space, one can superimpose IR tracers for grid cells that are
 211 separated spatially and recover the tendencies of the non-superimposed IR
 212 tracers from the tendencies of the superimposed IR tracers. That is, the
 213 tendencies $\overline{\mathcal{L}(\boldsymbol{\delta}^i)}$ and $\overline{\mathcal{L}(\boldsymbol{\delta}^j)}$ can be recovered from $\overline{\mathcal{L}(\boldsymbol{\delta}^i + \boldsymbol{\delta}^j)}$ if i and j are
 214 sufficiently separated spatially. This principle can be used to superimpose IR
 215 tracers for many grid cells into a single tracer, so that the $\overline{\mathcal{L}(\boldsymbol{\delta}^j)}$ terms can be
 216 computed with fewer tracers than would be used in the naïve implementation.
 217 We use this approach to compute the $\overline{\mathcal{L}(\boldsymbol{\delta}^j)}$ terms for the lateral mixing
 218 terms of $\mathbf{Q}$. The locality of this operator allows these terms to be computed
 219 with ≈ 30 IR tracers.

220 The IR tracer approach described above can also be used to compute the
 221 $\overline{\mathcal{L}(\boldsymbol{\delta}^j)}$ terms of $\mathbf{Q}$ for the advective operator. However, this would require

more IR tracers, because the advective operator in our ocean model has a wider computational stencil than the lateral mixing operator. So we have opted to use a less computationally demanding, though model specific, approach for the advective terms of $\mathbf{Q}$. Because the advective operator, denoted by $\mathcal{A}$, is linear with respect to tracer concentrations, we have

$$\frac{\partial \overline{\mathcal{A}}(\mathbf{u}, \mathbf{c})}{\partial c^j} = \overline{\mathcal{A}(\mathbf{u}, \delta^j)}, \quad (20)$$

where $\mathbf{u}$ denotes the (time-varying) advecting velocity. However, because the tracer advection scheme used in our ocean model is upwind biased (Holland et al., 1998), the time-averaged advective operator is not equal to the advective operator obtained using time-averaged velocities. However, the time-averaged advective operator is equal to the sum of the advective operators obtained using the time-average of the positive and negative parts of the velocity. That is,

$$\begin{aligned} \overline{\mathcal{A}(\mathbf{u}, \delta^j)} &= \overline{\mathcal{A}(\mathbf{u}^+, \delta^j) + \mathcal{A}(\mathbf{u}^-, \delta^j)} \\ &= \mathcal{A}(\overline{\mathbf{u}^+}, \delta^j) + \mathcal{A}(\overline{\mathbf{u}^-}, \delta^j). \end{aligned} \quad (21)$$

Combining these equations, we have

$$\frac{\partial \overline{\mathcal{A}}(\mathbf{u}, \mathbf{c})}{\partial c^j} = \mathcal{A}(\overline{\mathbf{u}^+}, \delta^j) + \mathcal{A}(\overline{\mathbf{u}^-}, \delta^j). \quad (22)$$

We use this equality to compute the advective terms of $\mathbf{Q}$. We compute $\overline{\mathbf{u}^+}$ and $\overline{\mathbf{u}^-}$ online, and evaluate $\mathcal{A}(\overline{\mathbf{u}^+}, \delta^j)$ and $\mathcal{A}(\overline{\mathbf{u}^-}, \delta^j)$ offline, using an implementation of the model's $\mathcal{A}$ in the offline code that constructs $\mathbf{Q}$.

Vertical mixing in our ocean model is implemented implicitly in time, so the computational stencil for this operator spans the entire water column.

240 We do not use the IR tracer approach for these terms of $\mathbf{Q}$ because of this,
 241 as it would require many more IR tracers. Instead, we compute the time-
 242 average of the vertical mixing coefficients online and use these, along with
 243 an implementation of the model’s vertical difference operator, in the offline
 244 code that constructs $\mathbf{Q}$.

245 As described in Danabasoglu et al. (2012), our ocean model includes an
 246 overflow parameterization. In this parameterization, tracer values in an over-
 247 flow’s source region instantaneously affect tracer values in the corresponding
 248 entrainment and outflow regions. This non-local dependence between tracer
 249 values from spatially separated grid cells increases the band-width of the oth-
 250 erwise sparse $\mathbf{Q}$, which increases the fill-in when the matrix is factored for
 251 solving (see below). We have omitted these terms from $\mathbf{Q}$ and still achieved
 252 satisfactory rates of convergence.

253 The final terms needed in $\mathbf{Q}$ are the partial derivatives of the tracer
 254 source-sink tendencies with respect to the tracer concentrations. Because
 255 these tendencies do not in general depend on the tracer concentrations in a
 256 linear way, the IR tracer approach described above is not applicable. For
 257 tracers with simple source-sink terms, these derivatives can be computed
 258 directly with analytical derivatives of the source-sink terms. More generally,
 259 the derivatives can be approximated with finite difference approximations
 260 (i.e., evaluate the source-sink tendencies with perturbed and unperturbed
 261 tracer values and apply standard finite difference formulas). Some source-
 262 sink tendencies, like the setting of ideal age to zero in the surface layer, are not
 263 differentiable with respect to the tracer concentrations. For the derivatives
 264 of these terms, we replace the tendency with a differentiable approximation

265 and include the derivative of the replacement in $\mathbf{Q}$. We emphasize that
 266 this approximation is only used in the preconditioner for the Krylov solver,
 267 through its usage in $\mathbf{Q}$. The source-sink tendency in the online model is
 268 unchanged. For ideal age, we approximate the setting of ideal age to zero
 269 with a restoring to zero term, using a timescale of 1 hour.

270 Most of the terms of $\mathbf{Q}$ described above, such as those computed with the
 271 IR tracer approach and those that arise from linear source-sink terms, are
 272 independent of the tracer concentrations. Because of this, these terms can be
 273 computed once, for a given time interval t_0 to $t_0 + \Delta t$, and used repeatedly for
 274 all Newton and Krylov iterations. Non-linear tracer source-sink tendencies
 275 however, lead to terms in $\mathbf{Q}$ that depend on tracer concentrations. These
 276 terms need to be recomputed for each Newton iteration, as the tracer state
 277 changes from one Newton iteration to the next.

278 Once $\mathbf{Q}$ is constructed, computing the matrix-vector product $\mathbf{P}_n \mathbf{v}$ in-
 279 volves solving the system of linear equations in Eq. (16) and applying Eq. (15).
 280 We refer the reader to Appendix C for the details on how we utilize the li-
 281 brary SuperLU-DIST (Li et al., 1999; Li and Demmel, 2003) to solve Eq. (16).

282 *2.4. Experiment Description*

283 The Newton-Krylov solver described above spins up tracers with re-
 284 spect to the model’s circulation over a time interval t_0 to $t_0 + \Delta t$. In
 285 our experiments, we have applied the solver to spin up the tracer ideal age
 286 (Thiele and Sarmiento, 1990). The ideal age of a water parcel is defined as
 287 the duration of time since the parcel was last in contact with the sea surface.
 288 The tracer ideal age is set to zero in the surface layer at every model time
 289 step and has a source term of 1 yr yr^{-1} in the ocean interior. We spun up

290 ideal age with respect to the model’s circulation over one-year intervals at
 291 multiple times in a 1000-year long NY forced physics run. One year was
 292 chosen because at this model resolution, the one-year period of the NY forc-
 293 ing leads to circulation that is approximately periodic with the same period.
 294 Longer durations would be appropriate for circulation fields with interannual
 295 variability, whether it is externally forced or internally generated. The tracer
 296 spin-ups were performed at multiple points along the physics run in order
 297 to evaluate how the duration of the physics run, i.e., how equilibrated the
 298 circulation is, affects the corresponding spun-up tracer solution. The ocean
 299 model in the physics run was started at a state of rest; temperature and
 300 salinity were initialized from the January-mean of the Polar Science Center
 301 Hydrographic Climatology (PHC2), which is constructed using data from
 302 Levitus et al. (1998), blending in data from Steele et al. (2001) for the Arc-
 303 tic Ocean. The spin-ups of ideal age were performed at multiple points in
 304 time in the physics run, at 50-year intervals up to year 500 of the physics run,
 305 and 100-year intervals from there up to year 1000. We performed one-year
 306 runs at each of these times to generate diagnostic output necessary to apply
 307 the preconditioner for the Krylov solver (see Section 2.3).

308 **3. Results**

309 We now present results of the applying to Newton-Krylov solver, which
 310 is using Eq. (7) to find a solution to Eq. (3), to the experimental framework
 311 described above.

3.1. Convergence of Solver

Our first test of the solver is to confirm that $\|\mathbf{G}(\mathbf{c}_n)\| \rightarrow 0$ as n increases, where $\|\mathbf{G}(\mathbf{c}_n)\|$ is the global, volume weighted root-mean-square change in ideal age over the year of integration. We do this initial verification in two separate runs of the solver, using the circulation from years 250 and 500 of the physics run (Fig. 1a). In these solver runs, the first Newton iterate, $\mathbf{c}_0$, for ideal age was all zeros and the Krylov solver was hard-coded to use four iterations. After a few Newton iterations, $\|\mathbf{G}(\mathbf{c}_n)\|$ decreases exponentially with n , verifying convergence. The rate of convergence is similar for the different years of circulation. We note that in both of these runs of the solver, the Armijo adjustment (Appendix A) to the Newton increment was invoked once for $n = 0$, and was not necessary for subsequent Newton iterations.

Another metric of convergence is that the fraction of the ocean’s volume where $|\mathbf{G}(\mathbf{c}_n)|$ exceeds a particular threshold should decrease to 0 as n increases. For ideal age, we use a threshold of 10^{-2} yrs/yr (Fig. 1b). This threshold is comparable to the natural abiotic radiocarbon equilibrium criterion in the Ocean Carbon Model Intercomparison Project, phase 2 (OCMIP2) protocol, which stated that 98% of the ocean volume should have a drift less than 10^{-3} permil/yr (Orr et al., 2000). In our convergence test runs, the fraction of the ocean’s volume where the change in ideal age exceeds our threshold decreases exponentially with n , verifying convergence. The fraction of the ocean’s volume below our threshold drops below 2% after five Newton iterations.

Another way of examining this convergence is to visualize the volume weighted histogram of $\log_{10} |\mathbf{G}(\mathbf{c}_n)|$. We do this for two different values of

337 n in the convergence test runs using the circulation from year 250 of the
 338 physics run (Fig. 2). An advantage of these histograms over the depiction
 339 of global measures in Fig. 1 is the additional information on the distribu-
 340 tion of $\log_{10} |\mathbf{G}(\mathbf{c}_n)|$ that is provided (e.g., mean, spread, and extent of
 341 the distribution’s tails). The histograms indicate that $|\mathbf{G}(\mathbf{c}_n)|$ is approx-
 342 imately log-normally distributed. Consistent with convergence, the mean
 343 of $\log_{10} |\mathbf{G}(\mathbf{c}_n)|$ decreases with n . Additionally, the standard deviation in-
 344 creases with n , though at a much smaller rate than the decrease in the mean.

345 *3.2. Stability of Simulations Initialized with Spun-up Tracers*

346 As alluded to in Section 1, one of the motivations for spinning up ocean
 347 tracers is to initialize simulations. We evaluate the utility of the Newton-
 348 Krylov solver for this purpose with two 10-year long experiments, initializing
 349 ideal age with one of the spun-up states described above. The ocean model’s
 350 physical state was initialized to the beginning of year 250 from the physics
 351 run. Ideal age was initialized to the state obtained with 5 Newton itera-
 352 tions using the circulation of year 250. In the first experiment, the ocean
 353 model’s physical state was reset at the end of every year to its state from
 354 the beginning of year 250, causing the ocean’s circulation to repeat the year
 355 250 circulation 10 times. The purpose of this experiment is to evaluate how
 356 ideal age changes over multiple years, but with a circulation field identical to
 357 that used in the Newton-Krylov solver. The change in ideal age in this ex-
 358 periment (Fig. 3a) was comparable to its residuals after 5 Newton iterations
 359 (Fig. 2a). In the second experiment, the ocean model’s physical state was
 360 allowed to freely evolve, yielding drift and internally generated variability in
 361 the ocean circulation. The purpose of this experiment is to evaluate how

Figure 1: Convergence of the tracer ideal age across Newton iterates: (a) Volume weighted root-mean-square of $\mathbf{G}$ (see Eq. (3)), (b) Fraction of ocean's volume where $\mathbf{G}$ exceeds the threshold 10^{-2} yrs/yr. The Armijo adjustment was applied once in the first Newton iteration.

Figure 2: Volume weighted histogram of $\log_{10} |\mathbf{G}(\mathbf{c}_n)|$ (see Eq. (3)): (a) Newton iteration 5, (b) Newton iteration 10. Ocean circulation was year 250 of the physics run.

the change in ideal age is impacted by this change in the ocean circulation away from that used in the Newton-Krylov solver. The change in ideal age in this experiment (Fig. 3b) was considerably larger than the residuals after 5 Newton iterations: only 42% of the ocean’s volume maintained change in ideal age below our threshold of 10^{-2} yrs/yr. However, the change was below a relaxed threshold of $5 \cdot 10^{-2}$ yrs/yr for 80% of the ocean’s volume.

An analogous pair of experiments were run where ideal age was initialized to the state obtained with 10 Newton iterations. The volume weighted histograms, not shown, portray results similar to those above. In the experiment with year 250 circulation repeating, change in ideal age was comparable to the residuals after 10 Newton iterations, demonstrating that for repeating circulation, the more converged solution maintains its state. In the experiment with freely evolving circulation, change in ideal age was larger and very similar to the change in the freely evolving circulation experiment initialized after 5 Newton iterations, demonstrating that for freely evolving circulation, the 5 additional Newton iterations have limited benefit.

3.3. Computational Performance

In the convergence test runs described in Section 3.1, our convergence criterion was reached with 5 Newton iterations, using a tracer distribution of all zeros as the initial Newton iterate. Each Newton iteration used 4 Krylov iterations, resulting in $5 \cdot 5 = 25$ evaluations of $\mathbf{G}$ and the same number of inversions of the Krylov preconditioner. In our implementation, solving the system of linear equations related to the preconditioner takes about the same number of CPU hours as running the ocean model with ideal age for 1 year. So running the Newton-Krylov solver to this convergence criterion

Figure 3: Volume weighted histogram of change in ideal age across a 10-year run in ideal age with spun-up ideal age used for initial state: (a) circulation repeats that used in ideal age spin-up, (b) circulation evolves freely over 10-year run. Ideal age was initialized from Newton iteration 5. The ocean physical state was initialized from year 250 of the physics run.

387 was computationally equivalent to running the ocean model with ideal age
 388 for 50 years. We project, using ideal age results from the physics run (not
 389 shown) that it would take over 10,000 years to reach this criterion using the
 390 brute force spin-up approach. So the Newton-Krylov solver is faster than
 391 the brute force spin-up approach by a factor over 200, even with an initial
 392 Newton iterate of all zeros. In practice, one would use a better initial Newton
 393 iterate. For instance, in our Newton-Krylov spin-ups using different years
 394 of circulation from the physics run (Section 3.4), we were able to satisfy
 395 the convergence criterion with 2 Newton iterations by using better initial
 396 Newton iterates, leading to the Newton-Krylov solver being faster than the
 397 brute force spin-up approach by a factor of over 500. In these applications
 398 of the solver, the initial ideal age iterate for a given year in the physics run
 399 was the spun-up ideal age from the preceding ideal age spin-up. This type of
 400 approach, initializing the spin-up with a previously spun-up solution, would
 401 be beneficial when evaluating the impact of a varying a model parameter on
 402 spun-up tracers.

403 *3.4. Dependence of Spun-up Tracer Concentrations on Duration of Physics* 404 *Run*

405 As an application of the solver, we have spun up ideal age at multiple time
 406 intervals in the long physics run. The resulting spun-up ideal age distribu-
 407 tions can be used to address questions that arise from different perspectives.
 408 One perspective is that of using ventilation tracers, like ideal age, as a tool
 409 to better understand the circulation of the ocean. From this perspective, the
 410 different spun-up ideal age distributions have the potential, through ideal
 411 age's integrative nature, to reveal aspects of the evolving model's circulation

412 that would not be readily apparent from examining only the temperature,
413 salinity, and velocity fields of the model. An example of a question that
414 arises from this perspective is: How is the ventilation of the ocean varying
415 as the density field of the model adjusts on long timescales? Another per-
416 spective is that of using the solver to spin up tracers for the purpose of using
417 or understanding the spun-up tracers themselves, not necessarily as a tool
418 to understand the ocean’s circulation. An example of a question that arises
419 from this perspective is: How long does physics run need to be in order for
420 the corresponding spun-up tracers to be robust? In the following, we are
421 focusing on this latter perspective.

422 The circulation in the long physics run has drift that persists for the
423 duration of the run. As the circulation drifts, the corresponding spun-up
424 ideal age values coevolve. In the following, we refer to this evolution of the
425 spun-up ideal age values as drift. We now describe how these spun-up ideal
426 age values, and their drift, depend on the duration of the physics run, i.e.,
427 how equilibrated the circulation is. We first examine zonal means of ideal
428 age at 35°N in the Pacific and Atlantic basins as a function of the year in the
429 physics run to which ideal age is spun up with respect to (Fig. 4). After the
430 physics run has been run for a sufficiently long duration, the corresponding
431 spun-up ideal age stabilizes, and becomes essentially constant as the physics
432 run is extended. In the Pacific zonal mean, this occurs for ideal age in the
433 top 750 m after a few hundred years. For instance, in the top 750 m, ideal
434 age is within 10% of its year 1000 values by year 450. In the older waters of
435 the deep Pacific, the drift in the spun-up ideal age values persists for the full
436 duration of the physics run. At year 1000 of the physics run, the derivative

437 of the spun-up ideal age with respect to the physics run year exceeds 0.25
 438 yrs/yr at all depths deeper than 2500 m. Spun-up ideal age at 35°N in the
 439 Atlantic stabilizes more quickly than in the Pacific; it is within 10% of its
 440 year 1000 values by year 600 at all depths. Its drift is below the threshold
 441 of $5 \cdot 10^{-2}$ yrs/yr at all depths shallower than 2000 m by year 450 and all
 442 depths shallower than 3000 m by year 700.

443 As mentioned above, a question that arises from the perspective that
 444 we are focusing on is: How long does physics run need to be in order for
 445 the corresponding spun-up tracers to be robust? We quantify this for zonal
 446 means of ideal age in the Pacific and Atlantic basins by computing, for each
 447 grid point, the time after which the relative drift in spun-up ideal age is below
 448 the threshold of $2 \cdot 10^{-4}$ yrs/yr² (Fig. 5). Relative drift is the derivative of the
 449 spun-up ideal age with respect to the physics run year divided by the spun-
 450 up ideal age. We use this relative drift criterion here because it seems to us
 451 to be of more practical use for ideal age than the OCMIP2 related absolute
 452 drift criterion. In the Pacific zonal mean, this threshold is reached by year
 453 900 of the physics run for much of the basin. Shallower than 4000 m, this
 454 threshold is reached in most of the southern hemisphere by year 500. In the
 455 Atlantic zonal mean, this threshold is reached by year 800 of the physics run
 456 for much of the basin south of 60°N. Shallower than 2000 m, this threshold
 457 is reached in most of the southern hemisphere by year 500.

458 It is likely that the duration required for the physics run depends on the
 459 physical parameterizations of the ocean model and the model's state at the
 460 beginning of the physics run, so the timescales described above should not
 461 be considered universal, even for a specific tracer, like ideal age. An alter-

native approach to determining how long the physics run needs to be is to functionally relate spun-up tracer values to diagnostics of the ocean model’s circulation. One could then run the physics run until these circulation diagnostics have small drift. It is fair to hope that such relationships would be applicable to ocean models with different physical parameterizations. While determining such relationships is not straightforward, intuition about the ocean’s circulation can suggest relationships to examine. For example, it is reasonable to expect that ideal age in the deep north Pacific is inversely related to volumetric transport into the deep Pacific from the south. Indeed, in our experiments, spun-up ideal age averaged across the Pacific at 3500 m and 45°N is inversely proportional to the modeled transport integrated from 3500 m to 5500 m across the Pacific at 35°S (Fig. 6).

4. Discussion

4.1. Tracer Spin-up Definition

In Section 2, we introduced Eq. (3) as our definition of the tracer spin-up problem. This definition is intuitive when the ocean model’s circulation is periodic with period Δt . However, it is not clear how appropriate this definition is when the circulation is not periodic (e.g., when the surface forcing has interannual variability or the ocean model has high enough spatial resolution to support internally generated variability). In our experience with using the Newton-Krylov solver in the presence of interannually varying circulation, not shown here, the Newton-Krylov solver does converge to a solution of Eq. (3). However, this solution is only useful (e.g., for initializing runs) if the circulation over the time interval t_0 to $t_0 + \Delta t$ is representative of the circula-

Figure 4: Zonal mean of spun-up ideal age at 35°N as function of physics run year used in the spin-up of ideal age: (a) Pacific basin, (b) Atlantic basin.

Figure 5: Duration of physics run needed to ensure that relative drift in the zonal mean of the spun-up ideal age is below the threshold of $2 \cdot 10^{-4}$ yrs/yr²: (a) Pacific basin, (b) Atlantic basin.

Figure 6: Inverse of zonal mean across the Pacific of spun-up ideal age at 45°N and depth of 3500 m vs. northward volumetric flux (Eulerian and bolus) integrated from 3500 m to 5500 m across the Pacific at 35°S.

486 tion over longer timescales. If the sampled circulation is not representative,
 487 and is anomalous in some way (e.g., deep water formation is uncharacteristi-
 488 cally high), then this anomalous circulation is reflected in the spun-up tracers.
 489 We have found that if the sampled circulation is long enough, and hence rep-
 490 resentative, then the solution produced by the Newton-Krylov solver is useful
 491 in the sense that tracer drift in simulations initialized with the corresponding
 492 spun-up tracers is small. An alternative approach to handling non-periodic
 493 circulation is to modify Eq. (3) in a way that reflects the non-periodic nature
 494 of the circulation (e.g., to compute the end-state minus start-state tracer dif-
 495 ference in water mass coordinates instead of Eulerian coordinates). We have
 496 not pursued such alternative approaches to extend the solver to non-periodic
 497 circulation.

498 *4.2. Stability of Simulations Initialized with Spun-up Tracers*

499 In Section 3.2, we showed that tracer drift is small in simulations ini-
 500 tialized with tracers that were spun up using the Newton-Krylov solver.
 501 In simulations repeatedly using the same circulation that was used in the
 502 Newton-Krylov solver, tracer drift remained similar to the Newton-Krylov
 503 residuals. From this, and the convergence results in Section 3.1, we conclude
 504 that the Newton-Krylov solver is working properly. In simulations using a
 505 circulation that evolved away from the circulation used in the Newton-Krylov
 506 solver, tracer drift was larger and essentially independent of how converged
 507 the Newton-Krylov solution was. We conclude that the additional drift,
 508 above the Newton-Krylov residuals, is due to the changes in the freely evolv-
 509 ing circulation. We glean two lessons from these results. The first is that
 510 when applying the Newton-Krylov solver to spin up tracers for initializing

511 simulations, it is important to use a circulation field in the solver iterations
 512 that is representative of the circulation of the simulations being initialized.
 513 For example, the change in circulation over years 250 to 260 with NY forcing
 514 was sufficient to induce non-trivial change in ideal age. So if one’s objective
 515 were to have minimal change in ideal age over that 10-year period, it would
 516 be better to use the Newton-Krylov solver with $\Delta t = 10$ years. As alluded
 517 to in Section 4.1, this point is particularly relevant for circulation fields with
 518 interannual variability, that it is important to use a representative period
 519 of circulation in that situation. The second lesson is that if the circulation
 520 field used in the solver does differ from the circulation that is ideal for the
 521 application at hand, one need not choose a solver convergence criterion that
 522 is tighter than the anticipated drift from the mismatch in circulation.

523 *4.3. Computational Performance*

524 We documented, in Section 3.3, the substantial performance benefit that
 525 the Newton-Krylov offers compared to the brute force spin-up approach.
 526 However, it is fair to point out that if the ocean model’s circulation field
 527 has interannual variability, then these speed-up factors decrease, because the
 528 cost of evaluating $\mathbf{G}$ increases. That said, the cost of solving the system of
 529 linear equations related to the preconditioner would not change. If evaluating
 530 $\mathbf{G}$ involved running the ocean model 10 years, and one had a good initial
 531 Newton iterate, then we estimate that our Newton-Krylov solver would be
 532 faster than the brute force spin-up approach by a factor of over 100.

533 4.4. *Dependence of Spun-up Tracer Concentrations on Duration of Physics* 534 *Run*

535 The results in Section 3.4 demonstrate that it may be necessary to run
536 the physics run many centuries in order to ensure robust application of the
537 Newton-Krylov solver for tracers. While these results are disappointing, it
538 is worth noting that the physics run need not include the tracers to which
539 the Newton-Krylov solver is applied. For tracer modules with many tracers,
540 this yields substantial savings in the computational cost in the physics run.
541 Moreover, we hypothesize that the weak ventilation bias in our ocean model’s
542 circulation may be increasing the required duration of the physics run. The
543 results for ideal age in Section 3.4 and natural abiotic radiocarbon, not shown,
544 indicate that the deep overturning circulation in the Pacific is sluggish early
545 in the physics run. We hypothesize that this anemic ventilation causes the
546 model predicted density structure to drift away from observations, which in
547 turn further reduces the ventilation, and that this feedback contributes to the
548 long duration that is required for the physics run in order to achieve robust
549 spun-up tracers. A prediction that arises from this hypothesis is that if the
550 model parameterizations were to achieve more realistic ventilation, then the
551 physics run would not need to be so long in order to achieve robust spun-up
552 tracer concentrations.

553 Another approach to reduce the computational time for the physics run is
554 to extend the Newton-Krylov solver to the active tracers of the ocean model.
555 While we have not done this, we speculate that the main challenge that
556 would arise in directly applying the technique to the active tracers would be
557 constructing a preconditioner that is both feasible to invert and adequately

558 represents how the model’s circulation, advection and mixing, depends upon
 559 the active tracers. We note that Bernsen et al. (2008) have applied Newton-
 560 Krylov solvers to a spin up a geostrophic ocean model, and Bernsen et al.
 561 (2010) have done so for a simplified configuration of version 4 of the Modular
 562 Ocean Model (MOM4).

563 *4.5. Implementing the Solver in Different Ocean Models*

564 It is of practical interest to apply the Newton-Krylov solver that we have
 565 developed to other ocean models (e.g., besides POP2). We first point out the
 566 advice of Kelley (2003), that it is preferable to use an existing Newton-Krylov
 567 implementation instead of implementing your own. That said, some batch
 568 computing environments, such as ours, make this impractical. The following
 569 is intended as a guide for modellers in this situation. We briefly describe, from
 570 a bottom-up perspective, the tools that are necessary to implement the solver.
 571 These tools are shell scripts in our implementation, but any implementation
 572 that achieves the required functionality would suffice. We initially describe
 573 the tools needed for a non-preconditioned Newton-Krylov solver, and then
 574 separately describe the tools for the Krylov preconditioner. At the lowest
 575 level, the Newton-Krylov solver requires a tool to compute $\mathbf{G}(\mathbf{c}(t_0))$, Eq. (3),
 576 for an arbitrary initial tracer state $\mathbf{c}(t_0)$. Computing $\mathbf{G}$ involves running
 577 the model forward in time for duration Δt , and computing the difference
 578 between the tracer states $\mathbf{c}(t_0 + \Delta t)$ and $\mathbf{c}(t_0)$. The details of how to do
 579 this will vary for different ocean models and computing environments. The
 580 next requirement is a tool to apply Eq. (10) to compute the matrix-vector
 581 multiplications required by GMRES. With these two tools, one can follow
 582 Algorithm 9.4 of Saad (2003) to implement GMRES to solve for the increment

583 in Newton’s method, $\delta \mathbf{c}_n$. Then one applies Eqs. (7) and (A.1) to implement
 584 Newton’s method to solve for the spun-up tracers.

585 Computing matrix-vector multiplications with the preconditioner matrix
 586 involves solving a system of linear equation with the matrix $\mathbf{Q} = \Delta t \partial \bar{\mathbf{f}} / \partial \mathbf{c}$.
 587 The description of the construction of the $\mathbf{Q}$ in Section 2.3 is in general
 588 applicable to other ocean models. The primary tool necessary for this con-
 589 struction is an implementation of the IR tracers. It is also necessary to be
 590 able to generate diagnostic output of tracer tendencies for the IR tracers. We
 591 expect that it is straightforward for a knowledgeable modeller to implement
 592 such a tracer module in an ocean model that has flexible support for tracers.
 593 In order for the IR tracer approach to be practical, it is necessary to come
 594 up with a decomposition of the set of the model’s grid points into subsets
 595 such that each IR tracer from a given subset can be superimposed without
 596 their tendencies overlapping. We have done this for POP’s structured grid
 597 by superimposing IR tracers whose grid indices are offset from each other
 598 with a regularly spaced offset that is greater than POP’s operator’s stencil
 599 width. We expect that a more involved approach would be necessary for an
 600 ocean model on an unstructured grid. The IR tracer approach can be used
 601 to compute the terms of $\mathbf{Q}$ that are related to the ocean model’s circulation,
 602 using the diagnostic IR tracer tendencies and Eq. (19). A technical aspect of
 603 this process is mapping the IR tracer tendencies to the correct entry in the
 604 data structure of the sparse matrix. In order to do this, we first construct
 605 mappings between the model’s grid index space and the index space of the
 606 sparse matrix. The location of non-zero entries in $\mathbf{Q}$ are then given by the
 607 composition of these index mappings with the model’s grid cell adjacency

matrix. For structured grids, non-zero entries in this latter matrix correspond to offsets in the model’s grid index space. For unstructured grids, we presume that this latter matrix would be provided along with the model grid. The terms of $\mathbf{Q}$ that arise from tracer source-sink terms are more a function of the tracer dynamics than the underlying ocean model. The approaches we described in Section 2.3 for these terms are applicable to general ocean models.

4.6. Benefits of the Brute Force Spin-up Approach

We note that there can be useful information in the transient tracer solution generated using the brute force spin-up approach. For example, for ideal age with steady circulation, the transient tracer solution can be used to derive the boundary propagator (Hall and Haine, 2002). This information is not generated when the Newton-Krylov solver is used to directly solve for the spun-up tracers. For applications where this information is of interest, the Newton-Krylov solver presented here would not be an appropriate tool.

5. Conclusions

We have presented a Newton-Krylov solver to spin up tracers in an ocean model. That is, it solves Eq. (3) using Eqs. (6) and (7). We have shown that the Newton-Krylov solver converges to a solution of Eq. (3), that free running simulations initialized with the resulting spun-up tracer have small drift, and that the solver produces these spun-up tracers with orders of magnitude less computational time than the brute force spin-up approach. This demonstrates that the solver can be an effective tool for fast spin-up of ocean tracers.

632 We have also used the solver to spin up ideal age and natural abiotic ra-
633 diocarbon to initialize coupled model simulations with CESM and to evaluate
634 parameterizations being considered for version 2 of CESM. We are actively
635 working on extending the solver to biogeochemical tracer modules, where
636 non-linearities in tracer source-sink terms necessitate enhancements to the
637 solver. Beyond biogeochemical tracers, we plan to extend the solver to the
638 ocean model’s active tracers, temperature and salinity.

639 **Appendix A. Description of the Newton-Krylov Solver Implemen-** 640 **tation**

641 Quality implementations of Newton-Krylov solvers are available. For ex-
642 ample, Kelley’s `nsoli.m` (Kelley, 2003) is an implementation in MATLAB, and
643 KINSOL (Collier et al., 2015) is a distributed memory parallel implementa-
644 tion applicable to larger problems. However, to the best of our knowledge,
645 these implementations, and others that we are aware of, require that the
646 solver remain in memory for the duration of the solve. This is problematic
647 in our batch computing environment for the following reasons. Evaluating
648 $\mathbf{G}$, the function whose root we are trying to find, for the model configuration
649 described in Section 2.2, takes $\approx 1/2$ an hour for the ideal age tracer and
650 $\Delta t = 1$ year. This evaluation time increases linearly with increasing Δt . It
651 also increases with increasing tracer count, i.e., when there is more than one
652 tracer being simultaneously spun up. In our batch computing environment,
653 large-scale computing jobs have a wall-clock limit of 12 hours. This places
654 a restrictive upper limit on how many times $\mathbf{G}$ can be evaluated in a single
655 job submission. For example, if one were spinning up the ideal age tracer

with respect to a circulation field that has interannual variability, and used $\Delta t = 8$ years, then only 3 $\mathbf{G}$ evaluations would be possible in a single batch submission. This makes it impractical to use one of these existing solvers out of the box.

We have instead implemented our own Newton-Krylov solver. In our implementation, we have split the solver into small callable pieces whose individual run times fit within the constraints of our batch computing environment. A light-weight driver, which can run outside of the wall-clock restrictions, manages the calling of the components of the solver. Quantities that would persist in memory in the out-of-the-box solvers, such as basis vectors of the Krylov solver, function evaluations, and intermediate coefficients from the solver, are stored in files.

Our implementation of Newton’s method is fairly simplistic. We compute the Newton increment $\delta \mathbf{c}_n$, defined by Eq. (6), using the Krylov solver. Then, following (Kelley, 2003, Section 1.6), we find the smallest integer $m \geq 0$ such that

$$\|\mathbf{G}(\mathbf{c}_n + 2^{-m}\delta \mathbf{c}_n)\| < (1 - \alpha 2^{-m}) \|\mathbf{G}(\mathbf{c}_n)\|, \quad (\text{A.1})$$

where $\|\cdot\|$ is the volume weighted root-mean-square norm, and set $\mathbf{c}_{n+1} = \mathbf{c}_n + 2^{-m}\delta \mathbf{c}_n$. This condition, Eq. (A.1), referred to by Kelley (2003) as the Armijo rule, ensures that the solver is making a sufficient decrease in $\|\mathbf{G}\|$. Following Kelley (2003), we use $\alpha = 10^{-4}$. We have used this simple line search method instead of one of the more sophisticated methods described in Kelley (2003) because of the relatively high computational cost of evaluating our $\mathbf{G}$.

Our implementation of preconditioned GMRES follows Algorithm 9.4 of

680 Saad (2003). Dot products of vectors are used throughout GMRES (e.g., to
681 compute projections and to normalize vectors). Consistent with $\|\cdot\|$ being the
682 volume weighted root-mean-square norm, dot products of vectors of tracer
683 concentrations are defined as volume weighted sums of tracer products. In
684 our application of Eq. (10) to compute the matrix-vector multiplications
685 required by GMRES, we normalize $\|\delta\mathbf{c}\| = 1$ and set $\sigma = .5 \cdot 10^{-3}$. We
686 have not investigated the sensitivity of the solver to the selection of σ . It
687 is possible that tracers with more complicated dynamics than ideal age will
688 require a more refined approach for the selection of σ , such as the method
689 described in (Kelley, 2003, Section 3.2.1).

690 Appendix B. Derivation of Krylov Preconditioner

691 We present here the differential and algebraic manipulations that lead
692 from Eq. (13) to Eq. (14). Differentiating both sides of Eq. (13) with respect
693 to $\mathbf{c}(t_0)$ yields

$$\frac{\partial \tilde{\Phi}}{\partial \mathbf{c}(t_0)} - \mathbf{I} = \Delta t \frac{\partial \bar{\mathbf{f}}}{\partial \mathbf{c}} \frac{\partial \tilde{\Phi}}{\partial \mathbf{c}(t_0)}, \quad (\text{B.1})$$

694 where $\mathbf{I}$ is the identity matrix. Rearranging this to solve for $\partial \tilde{\Phi} / \partial \mathbf{c}(t_0)$ yields

$$\frac{\partial \tilde{\Phi}}{\partial \mathbf{c}(t_0)} = \left(\mathbf{I} - \Delta t \frac{\partial \bar{\mathbf{f}}}{\partial \mathbf{c}} \right)^{-1}. \quad (\text{B.2})$$

695 This enables the following algebraic manipulations to derive Eq. (14):

$$\begin{aligned} \mathbf{P}_n &= \tilde{\mathbf{J}}^{-1} = \left(\frac{\partial \tilde{\mathbf{G}}}{\partial \mathbf{c}(t_0)} \right)^{-1} = \left(\frac{\partial \tilde{\Phi}}{\partial \mathbf{c}(t_0)} - \mathbf{I} \right)^{-1} \\ &= \left(\left(\mathbf{I} - \Delta t \frac{\partial \bar{\mathbf{f}}}{\partial \mathbf{c}} \right)^{-1} - \mathbf{I} \right)^{-1} = \left(\Delta t \frac{\partial \bar{\mathbf{f}}}{\partial \mathbf{c}} \right)^{-1} - \mathbf{I}, \end{aligned} \quad (\text{B.3})$$

696 where we have made use of the following chain of matrix identities:

$$\begin{aligned}
& ((\mathbf{I} - \mathbf{M})^{-1} - \mathbf{I})^{-1} = ((\mathbf{I} - \mathbf{M})^{-1} - (\mathbf{I} - \mathbf{M})(\mathbf{I} - \mathbf{M})^{-1})^{-1} \\
& = (\mathbf{M}(\mathbf{I} - \mathbf{M})^{-1})^{-1} = (\mathbf{I} - \mathbf{M})\mathbf{M}^{-1} = \mathbf{M}^{-1} - \mathbf{I}. \quad (\text{B.4})
\end{aligned}$$

697 Appendix C. Utilizing SuperLU_DIST

698 As stated in Section 2.3, once we construct the matrix $\mathbf{Q} = \Delta t \partial \bar{\mathbf{f}} / \partial \mathbf{c}$, we
699 use SuperLU_DIST to solve the system of linear equations in Eq. (16). As its
700 name suggests, SuperLU_DIST does this by first constructing an LU decom-
701 position of the matrix $\mathbf{Q}$ and then using forward and backward substitution
702 to directly solve the factored systems of linear equations. The DIST suffix
703 denotes that we are using the distributed memory version of the library. We
704 are using the parallel symbolic factorization functionality in SuperLU_DIST
705 (Grigori et al., 2007). Compared to the serial version, the parallel version
706 significantly reduces the time and memory usage of the symbolic factoriza-
707 tion step of constructing the LU decomposition. A drawback of our batch
708 computing environment is that the queue wall-clock limits preclude us from
709 keeping the LU decomposition in memory, once it is constructed. Because
710 SuperLU_DIST does not have the ability to store the LU decomposition to
711 disk, we end up recreating it every iteration of the Krylov solver. Using a
712 sparse matrix library that has the ability to store the factored matrix to disk
713 would perhaps improve the overall computational efficiency of our Newton-
714 Krylov solver.

715 **Acknowledgments**

716 The National Center for Atmospheric Research is sponsored by the Na-
717 tional Science Foundation. This work was supported in part by the Depart-
718 ment of Energy, Office of Science, Biological and Environmental Research,
719 under SciDAC award number DE-SC0006768. Computing resources were
720 provided by the Climate Simulation Laboratory at NCAR’s Computational
721 and Information Systems Laboratory (CISL), sponsored by the National Sci-
722 ence Foundation and other agencies. The CESM project is supported by the
723 National Science Foundation and the Office of Science (BER) of the U.S.
724 Department of Energy. We thank François Primeau, Matthew Long, Frank
725 Bryan, and three anonymous reviewers for their constructive comments.

726 **References**

- 727 Bardin, A., Primeau, F., Lindsay, K., 2014. An offline implicit solver for
728 simulating prebomb radiocarbon. *Ocean Model.* 73, 45–58.
- 729 Bardin, A., Primeau, F., Lindsay, K., Bradley, A., 2016. Evaluation of the
730 accuracy of an offline seasonally-varying matrix transport model for simu-
731 lating ideal age. *Ocean Model.* 105, 25–33.
- 732 Bernsen, E., Dijkstra, H. A., Thies, J., Wubs, F. W., 2010. The application of
733 Jacobian-free Newton-Krylov methods to reduce the spin-up time of ocean
734 general circulation models. *J. Comput. Phys.* 229 (21), 8167–8179.
- 735 Bernsen, E., Dijkstra, H. A., Wubs, F. W., 2008. A method to reduce the
736 spin-up time of ocean models. *Ocean Model.* 20 (4), 380–392.

737 Collier, A. M., Hindmarsh, A. C., Serban, R., Woodward,
738 C. S., July 2015. User documentation for KINSOL v2.8.2.
739 Tech. Rep. UCRL-SM-208116, Center for Applied Scien-
740 tific Computing, Lawrence Livermore National Laboratory,
741 http://computation.llnl.gov/casc/sundials/documentation/kin_guide.pdf.

742 Danabasoglu, G., Bates, S. C., Briegleb, B. P., Jayne, S. R., Jochum, M.,
743 Large, W. G., Peacock, S., Yeager, S. G., 2012. The CCSM4 ocean com-
744 ponent. *J. Climate* 25 (5), 1361–1389.

745 Danabasoglu, G., Large, W. G., Briegleb, B. P., 2010. Climate impacts of
746 parameterized Nordic Sea overflows. *J. Geophys. Res.* 115 (C11).

747 DeVries, T., Primeau, F., 2011. Dynamically and observationally constrained
748 estimates of water-mass distributions and ages in the global ocean. *J. Phys.*
749 *Oceanogr.* 41 (12), 2381–2401.

750 Gent, P. R., McWilliams, J. C., 1990. Isopycnal mixing in ocean circulation
751 models. *J. Phys. Oceanogr.* 20 (1), 150–155.

752 Grigori, L., Demmel, J. W., Li, X. S., 2007. Parallel symbolic factorization for
753 sparse LU with static pivoting. *SIAM J. Sci. Comput.* 29 (3), 1289–1314.

754 Hall, T. M., Haine, T. W. N., 2002. On ocean transport diagnostics: The
755 idealized age tracer and the age spectrum. *J. Phys. Oceanogr.* 32 (6), 1987–
756 1991.

757 Holland, M. M., Bailey, D. A., Briegleb, B. P., Light, B., Hunke, E., 2012.
758 Improved sea ice shortwave radiation physics in CCSM4: The impact of
759 melt ponds and aerosols on Arctic sea ice. *J. Climate* 25 (5), 1413–1430.

760 Holland, W. R., Chow, J. C., Bryan, F. O., 1998. Application of a third-order
761 upwind scheme in the NCAR ocean model. *J. Climate* 11 (6), 1487–1493.

762 Holzer, M., Primeau, F. W., 2010. Improved constraints on transit time
763 distributions from argon 39: A maximum entropy approach. *J. Geophys.*
764 *Res.* 115 (C12).

765 Hunke, E. C., Lipscomb, W. H., 2008. CICE: The Los Alamos Sea Ice Model,
766 documentation and software user’s manual, version 4.0. Tech. Rep. LA-CC-
767 06-012, Los Alamos National Laboratory, Los Alamos, NM.

768 Hurrell, J. W., Holland, M. M., Gent, P. R., Ghan, S., Kay, J. E., Kushner,
769 P. J., Lamarque, J.-F., Large, W. G., Lawrence, D., Lindsay, K., Lip-
770 scomb, W. H., Long, M. C., Mahowald, N., Marsh, D. R., Neale, R. B.,
771 Rasch, P., Vavrus, S., Vertenstein, M., Bader, D., Collins, W. D., Hack,
772 J. J., Kiehl, J., , Marshall, S., 2013. The Community Earth System Model:
773 A framework for collaborative research. *Bull. Amer. Meteor. Soc.* 94 (9),
774 1339–1360.

775 Kelley, C. T., 2003. Solving Nonlinear Equations with Newton’s Method.
776 Society for Industrial and Applied Mathematics, Philadelphia, PA.

777 Khatiwala, S., 2008. Fast spin up of ocean biogeochemical models using
778 matrix-free Newton-Krylov. *Ocean Model.* 23 (3–4), 121–129.

779 Khatiwala, S., Primeau, F., Holzer, M., 2012. Ventilation of the deep ocean
780 constrained with tracer observations and implications for radiocarbon es-
781 timates of ideal mean age. *Earth Planet. Sci. Lett.* 325–326, 116–215.

782 Khatiwala, S., Visbeck, M., Cane, M. A., 2005. Accelerated simulation of
783 passive tracers in ocean circulation models. *Ocean Model.* 9 (1), 51–69.

784 Large, W. G., McWilliams, J. C., Doney, S. C., 1994. Oceanic vertical mixing:
785 A review and a model with a nonlocal boundary layer parameterization.
786 *Rev. Geophys.* 32 (4), 363–403.

787 Large, W. G., Yeager, S. G., 2004. Diurnal to decadal global forcing for ocean
788 and sea-ice models: The data sets and flux climatologies. Tech. Rep. TN-
789 460+STR, NCAR.

790 Levitus, S., Boyer, T., Concright, M., Johnson, D., O’Brien, T., Antonov, J.,
791 Stephens, C., Garfield, R., 1998. World Ocean Database 1998, Volume 1:
792 Introduction. NOAA Atlas NESDIS 18, U.S. Government Printing Office,
793 Washington, D.C., p. 346.

794 Li, X., Primeau, F. W., 2008. A fast Newton-Krylov solver for seasonally
795 varying global ocean biogeochemistry models. *Ocean Model.* 23 (1–2), 13–
796 20.

797 Li, X. S., Demmel, J. W., June 2003. SuperLU_DIST: A scalable distributed-
798 memory sparse direct solver for unsymmetric linear systems. *ACM Trans.*
799 *Math. Software* 29 (2), 110–140.

800 Li, X. S., Demmel, J. W., Gilbert, J. R., Grigori, L., Shao, M.,
801 Yamazaki, I., September 1999. SuperLU Users’ Guide. Tech.
802 Rep. LBNL-44289, Lawrence Berkeley National Laboratory,
803 <http://crd.lbl.gov/~xiaoye/SuperLU/>.

804 Orr, J., Najjar, R., Sabine, C., Joos, F., 2000. Abiotic-HOWTO. In-
805 ternal OCMIP report, LSCE/CEA Saclay, Gif-sur-Yvette, France,
806 <http://ocmip5.ipsl.jussieu.fr/OCMIP/phase2/simulations/Abiotic/HOWTO-Abiotic.htm>

807 Saad, Y., 2003. Iterative Methods for Sparse Linear Systems, 2nd Edition.
808 Society for Industrial and Applied Mathematics, Philadelphia, PA.

809 Saad, Y., Schultz, M. H., 1986. GMRES: A generalized minimal residual
810 algorithm for solving nonsymmetric linear systems. SIAM J. Sci. and Stat.
811 Comput. 7 (3), 856–869.

812 Smith, R., Jones, P., Briegleb, B., Bryan, F., Danabasoglu, G., Den-
813 nis, J., Dukowicz, J., Eden, C., Fox-Kemper, B., Gent, P., Hecht,
814 M., Jayne, S., Jochum, M., Large, W., Lindsay, K., Maltrud, M.,
815 Norton, N., Peacock, S., Vertenstein, M., Yeager, S., 2010. The
816 Parallel Ocean Program (POP) reference manual, ocean compo-
817 nent of the Community Climate System Model (CCSM). Tech. Rep.
818 LAUR-10-01853, Los Alamos National Laboratory, Los Alamos, NM,
819 <http://www.cesm.ucar.edu/models/cesm1.0/pop2/doc/sci/POPRefManual.pdf>.

820 Steele, M., Morley, R., Ermold, W., 2001. PHC: A global ocean hydrography
821 with a high-quality Arctic Ocean. J. Climate 14 (9), 2079–2087.

822 Thiele, G., Sarmiento, J. L., 1990. Tracer dating and ocean ventilation. J.
823 Geophys. Res. 95 (C6), 9377–9391.