Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

Technical Note: An efficient method for accelerating the spin-up process for process-based biogeochemistry models

Yang Qu[1], Shamil Maksyutov[2], and Qianlai Zhuang[1,3]

[1]Department of Earth, Atmospheric, and Planetary Sciences, Department of Agronomy, Purdue University, West Lafayette, IN 47907 USA

[2]National Institute for Environmental Studies, 16-2 Onogawa, Tsukuba, Ibaraki, 305-8506 Japan

[3]Department of Agronomy, Purdue University

Correspondence to: qzhuang@purdue.edu

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

Abstract

To better understand the role of terrestrial ecosystems in the global carbon cycle and their feedbacks to the global climate system, process-based biogeochemistry models need to be improved with respect to model parameterization and model structure. To achieve these improvements, the spin-up time for those differential equation-based models needs to be shortened. Here, an algorithm for a fast spin-up was developed and implemented in a biogeochemistry model, the Terrestrial Ecosystem Model (TEM). With the new spin-up algorithm, we showed that the model reached a steady state in less than 10 years of computing time, while the original method requires more than 200 years on average of model run. For the test sites with five different plant function types, the new method saves over 90% of the original spin-up time in site-level simulations. In North America simulations, average spin-up time saving for all grid cells is 85% for either daily or monthly version of TEM. The developed spin-up method shall greatly facilitate our future quantification of carbon dynamics at fine spatial and temporal scales.

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

1. Introduction

Biogeochemistry models contain state variables representing various pools of carbon and nitrogen and a set of flux variables representing the element and material transfers between different state variables. Model spin-up is a step to get biogeochemistry models to a steady state for those state and flux variables (McGuire et al., 1992; King, 1995; Johns et al., 1997; Dickinson et al., 1998). Spin-up normally uses cyclic forcing data to force the model run, and reach a steady state, which will be used as initial conditions for model transient simulations. The steady state is reached when modeled state variables show a cyclic pattern or a constant and often requires a significant amount of computation time, which needs to be accelerated for regional and global simulations at fine spatial and temporal scales.

Spin-up is normally achieved by running model repeatedly using one or several decades of meteorological or climatic data, until a steady state is reached. The step could require model repeatedly run for more than 2000 annual cycles. Specifically, the model will check the stability of the simulated carbon and nitrogen fluxes as well as state variables with specified threshold values. For instance, the model will check if the simulated annual net ecosystem production (NEP) is less than 1 g C m^{-2} yr^{-1} (McGuire et al. ,1992). Another method to reach a steady state is to obtain the analytical solutions (King et al, 1995; Comins, 1997), which might also take a significantly long time.

For different biogeochemistry models, spin-up could take hundreds and thousands of years to reach a stability, normally longer than the model projection period (Thornton et al., 2005). Therefore, a more efficient method to reach the steady state will speed up the entire model simulation. Recently, a semi-analytical method (Xia et al., 2012) has been adapted to a carbon-nitrogen coupled model to speed up the spin-up process. The idea is to get an analytical solution

very close to a steady condition, then start spin-up from the solution, which could significantly reduce spin-up time. However, this technique did not reach a cyclic pattern for state and flux variables and required an additional spin-up process to achieve the steady state.

Here we developed a new method to accelerate the spin-up process. We tested the method for representative plant function types and the North America with both daily and monthly versions of TEM (Zhuang et al., 2003). In addition, we compared the performance of our algorithms with the semi-analytical version of Xia et al. (2012). The new algorithms shall help us conduct very high spatial and temporal resolution simulations with process-based biogeochemistry models in the future.

2. Method

2.1 TEM description

We used a process-based biogeochemistry model, the Terrestrial Ecosystem Model (TEM; Zhuang et al. 2003) as testbed to demonstrate the performance of the new algorithms of spin-up. TEM simulates the dynamics of ecosystem carbon and nitrogen fluxes and pools (McGuire et al., 1992; Zhuang et al., 2010, 2003). It contains five state variables: carbon in living vegetation (C_v), nitrogen in living vegetation (N_v), organic carbon in detritus and soils (C_s), organic nitrogen in detritus and soils (N_s), and available inorganic soil nitrogen (N_{av}). Carbon and nitrogen dynamics in TEM are governed by following equations:

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

$$\frac{dC_v}{dt} = GPP - R_A - L_C \quad (1)$$

$$\frac{dN_v}{dt} = NUPTAKE - L_N \quad (2)$$

$$\frac{dC_s}{dt} = L_c - R_H \quad (3)$$

$$\frac{dN_s}{dt} = L_N - NETNMIN \quad (4)$$

$$\frac{dN_{av}}{dt} = NINPUT + NETNMIN - NLOST - NUPTAKE \quad (5)$$

Where GPP is gross primary production, R_A is autotrophic respiration, L_C is carbon in litterfall, $NUPTAKE$ is nitrogen uptake by vegetation, L_N is nitrogen in litterfall, R_H is heterotrophic respiration, $NETNMIN$ is net rate of mineralization of soil nitrogen, $NINPUT$ is nitrogen input from outside ecosystem, $NLOST$ is nitrogen loss from ecosystem. Key carbon fluxes are defined as:

$$GPP = C_{\max} f(PAR) f(PHENOLOGY) f(FOLIAGE) f(T) f(C_a, G_v) f(NA) f(FT) \quad (6)$$

$$NPP = GPP - R_A \quad (7)$$

$$NEP = GPP - R_A - R_H \quad (8)$$

NEP will be near zero when the ecosystem reaches a steady state. Therefore, the spin-up goal is to keep running the model driven with repeated climate forcing data until NEP is close to zero with a certain tolerance value (e.g., 0.1 g C m^{-2} yr^{-1}).

2.2 Spin-up acceleration method

TEM can be re-formulated as:

$$\frac{d\vec{x}}{dt} = g(\vec{x}) + \vec{h} \quad (9)$$

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

Where x is a vector of state variables (e.g., V_c); $\vec{h}$ is vector of carbon/nitrogen input from the atmosphere, independent on $\vec{x}$; g(x) is the process rate function of element pools (e.g., GPP).

By linearizing the model in term of pools, we could get:

$$g(\vec{x},t) = g(\vec{x}_0,t) + J(\vec{x} - \vec{x}_0) \quad \text{.....(10)}$$

Where J is the Jacobian matrix of the process rate:

$$J = \frac{dg}{dx} = \begin{bmatrix} \frac{\partial g_1}{\partial x_1} & \cdots & \frac{\partial g_1}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial g_n}{\partial x_1} & \cdots & \frac{\partial g_n}{\partial x_n} \end{bmatrix} \quad \text{.....(11)}$$

The numerical discretization of equation (9) is:

$$x_k - x_{k-1} = \tau \cdot J_{k-\frac{1}{2}} \cdot x_{k-1} + \tau\left(g\left(x_{0,k-1}\right) - J \cdot x_{0,k-1} + h_{k-1}\right) \quad \text{.....(12)}$$

Where τ is time step (month), x_k is pool size at time k, $J_{k-\frac{1}{2}}$ is a Jacobian matrix at time step $k - \frac{1}{2}$ (half timestep).

We introduce:

$$f_{k-1} = g\left(x_{0,k-1}\right) - J \cdot x_{0,k-1} + h_{k-1} \quad \text{.....(13)}$$

The equation can then be written as:

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

$$x_k - x_{k-1} = \tau \cdot J_{k-\frac{1}{2}} \cdot x_{k-1} + \tau \cdot f_{k-1} \quad (14)$$

Where $J_{k-\frac{1}{2}}$ is a Jacobian matrix at time step $k-\frac{1}{2}$ (half step). After running a large number of annual cycles, model approaches a cyclo-stationary state, which can be expressed by condition $x^{T+i} = x^i$, where T is the number of time steps in one cycle. For example, when spin up is made at monthly time step using monthly climatology of temperature, precipitation and other forcing data, T equals 12, and x^1 is the size of carbon pools on January 1st, while $J^{1.5}$ is the matrix of mean process rate constants for January.

By introducing

$$A_k = \tau \cdot J_{k-\frac{1}{2}},\ y_k = \tau f_{k-\frac{1}{2}},\ B_k = I,\ C_k = I + A$$

where I is an identity matrix.

Eq. (12) can be written as:

$$-C_k \cdot x_{k-1} + B_k \cdot x_k = y_k \quad (15)$$

The cyclic boundary condition is: $x_1 = x_{T+1}$

Then Eq. (13) will become:

$$-C_1 \cdot x_T + B_1 \cdot x_1 = y_1 \quad (15a)$$

Thus equations (15, 15a) become a formulation of a linear problem with T unknown vectors x_k, which can be solved using LU decomposition or Gaussian elimination. Xia et al (2012, see

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

Eq. 4) and Kwon and Primeau (2006) also had linear equations for a steady state, but only for annually averaged mean value. Going for annual average form reduces the size of problem, but prevents Xia et al (2012) from obtaining exact solution of the system (see their Eq. 3, 3a), because introducing cyclic boundary conditions in their Eq. (3a) was missing in their methods.

2.2 Numerical Implementation

Equation (15a) is explicitly expressed as:

$$\begin{pmatrix} B & 0 & 0 & 0 & 0 & 0 & -C \\ -C & B & 0 & 0 & 0 & 0 & 0 \\ 0 & -C & B & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & -C & B & 0 & 0 \\ 0 & 0 & 0 & 0 & -C & B & 0 \\ 0 & 0 & 0 & 0 & 0 & -C & B \end{pmatrix} \times \begin{pmatrix} x^1 \\ x^2 \\ \\ x^k \\ \\ x^t \end{pmatrix} = \begin{pmatrix} y^1 \\ \\ \\ \\ \\ y^t \end{pmatrix}, \quad \text{.....(16)}$$

Eq. (16) can be shown in form $Mx = Y$.

Apply the Gaussian elimination to upper block that reduces M to a lower triangular form and the elimination process is applied from right to left in the top row of M involving 2x2 blocks of matrices B, C, D and D'.

$$\begin{pmatrix} D^1 & D \\ -C_k & B_k \end{pmatrix} \begin{pmatrix} y_1 \\ y_k \end{pmatrix} \quad \text{.....(17)}$$

The result matrix is:

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

$$M' = \begin{pmatrix} B' & 0 & 0 & 0 & 0 & 0 & 0 \\ -C & B & 0 & 0 & 0 & 0 & 0 \\ 0 & -C & B & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & -C & B & 0 & 0 \\ 0 & 0 & 0 & 0 & -C & B & 0 \\ 0 & 0 & 0 & 0 & 0 & -C & B \end{pmatrix} \quad \text{.....(18)}$$

The solution of eq. (15a) will be readily obtained for x.

2.3 Algorithm implementation to TEM

In original TEM, carbon fluxes can be defined as:

$$NPP = GPP - MR - GR \text{.....(19)}$$

$$MR = V_C \cdot K_T \text{.....(20)}$$

$$GR = \begin{cases} 0.25 \cdot (GPP - MR), \ if\ GPP > MR \\ 0 \qquad\qquad\qquad , \ otherwise \end{cases} \text{.....(21)}$$

Where net primary production (NPP) is defined as the difference of GPP and plant maintenance respiration (MR) and growth respiration (GR). MR is assumed as a function of V_C and temperature (K_T). Here we revised MR calculation:

$$MR = \begin{cases} V_C \cdot K_T, \ if\ GPP > V_C \cdot K_T \\ 0.75 \cdot V_C \cdot K_T + 0.25 \cdot GPP, otherwise \end{cases} \text{.....(21)}$$

The net ecosystem production (NEP) is defined as the difference between NPP and heterotrophic respiration (R_H).

The basic workflow to implement the method is: 1) linearizing TEM first to get a sparse matrix with n-variable system; 2) performing Gaussian elimination for the linear system; 3) solving the sparse matrix to acquire the state variable values (Figure 1). To adapt this method to

a daily version of TEM, we changed the cyclic condition T from 12 to 365. The other steps are the same as monthly version. We tested the new method for carbon only version and carbon-nitrogen coupled version of TEM for different PFTs (Table 1). Specifically, for the carbon only version, we only solved the differential equations that govern the carbon dynamics, while for the carbon-nitrogen coupled version, we solved the differential equations that govern both carbon and nitrogen dynamics in the system. For the both versions, the spin-up process strives to reach a steady state for carbon pools and fluxes.

3. Results and Discussion

At Harvard Forest site, the traditional spin-up method took 564 years to get the steady state for both the carbon-only and coupled carbon–nitrogen simulations with annual NEP less than 0.1 g C m^{-2} yr^{-1} (Figure 2). The improved method took 72 years for the carbon only and 122 for the coupled carbon–nitrogen simulations, respectively. For carbon and nitrogen pools, it took another 45 years (equivalent cyclic time) to reach a steady state with NEP less than 0.1 g C m^{-2} yr^{-1}. In comparison with the traditional spin-up method (Zhuang et al., 2003), the new method saved 65% of computational time to get the steady state in the carbon-only simulations (Table 2). The differences in steady-state carbon pools between using the new method and traditional spin-up methods were small (less than 0.85%). Similarly, for the coupled carbon–nitrogen simulations, the new method saves a similar amount of time to reach the steady state. For the seven test sites, it takes on average 0.6 seconds using new method to reach a steady state. Compared to the original spin-up method, the new method is not only faster, but also computationally stable.

The time of spin-up to reach a steady state of NEP varied for different PFT grids using the original method (Figure 2). In general, to allow 98% grid cells reach their steady states of NEP,

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

it will take 250 annual model runs. While the new method will only need on average 0.6 seconds (equivalent to 60-year annual model runs with the original method) (Figure 3). For regional tests in North America, we found that the average saving time with the new method with monthly TEM is 25%, 32%, and 22%, for Alaska, Canada, and the conterminous US, respectively.

To compare the performance of the new method with other existing methods, we adapted the semi-analytical method (Xia et al., 2012) to TEM model. To do that, we first revised the TEM model structure to:

$$\frac{dP(t)}{dt} = \varepsilon ACP(t) \quad (22)$$

Where P(t) is a vector of pools in TEM (e.g., V_C and S_C). ε is a scalar. A is a pool transfer matrix (in which A_{ij} represents the fraction of carbon transfer from pool j to i). C is a diagonal matrix with pool components (where diagonal components quantify the fraction of carbon left from the state variables after each time step). With this method, we obtained an analytical solution for the intermediate state. We then kept running TEM with the traditional spin-up process. Specifically, we started TEM simulation to estimate the state variable values. Based on these values, the spin-up runs were conducted to reach the final steady state. We found that the semi-analytical solution is better than the original spin-up method, but slower than the new method proposed in this study (Table 2).

4. Summary

We developed a new method to speed up the spin-up process in process-based biogeochemistry models. We found that the new method shortened 90% of the spin-up time

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

using the traditional method. For regional simulations in North America, average spin-up time saving is 85% for either daily or monthly version of TEM. This method will significantly help our future carbon dynamics quantification with biogeochemistry models at fine spatial and temporal scales.

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

193 Table 1. Test sites for new spin-up algorithms

Site Name	Location	PFT	Reference
1. Fort Peck	48.3N, 105.1W	Grassland	Gilmanov et al. [2005]
2. Bartlett Exp Forest	44.1N, 71.3W	Deciduous broadleaf	Ollinger et al. [2005]
3. UCI_1850	55.9N, 98.5W	Evergrenn needle-leaf	Goulden et al. [2006]
4. Vaira Ranch	38.4N, 121.0W	Grassland	Baldocchi et al. [2004]
5. Missouri Ozark	38.7N, 92.2	Deciduous broadleaf	Gu et al. [2007, 2012]
6. Niwot Ridge	40.0N, 105.5W	Evergrenn needle-leaf	Turnipseed et al. [2003, 2004]
7. Harvard Forest	43.5N, 72.2W	Deciduous broadleaf	Van Gorsel et al. [2009]

194

195

196

197

198

199

200

201

202

203

204

205

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018

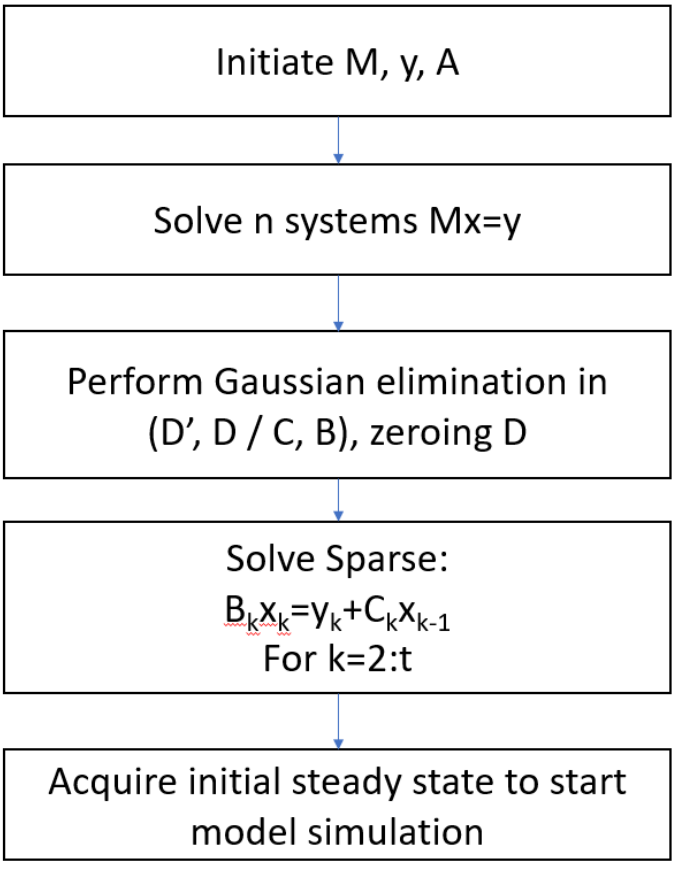
206 Table 2. Spin-up time comparison for different methods, seconds represent real computation time,

207 years refer to the spin-up annual cycles

Site No.	Original Spin-up Year	Spin-up computation time (Seconds)	New method computation time (Seconds)	Semi-analytical method (equivalent annual cycles
1	231	1.3	0.5	0.7s (+76)
2	305	1.7	0.3	0.8s (+101)
3	245	1.5	0.4	0.9s (+52)
4	443	2.2	0.4	0.5s (+118)
5	304	1.8	0.4	0.8s (+86)
6	204	1.1	0.3	0.7s (+43)
7	564	2.5	0.6	0.9(+45)

208

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018



209

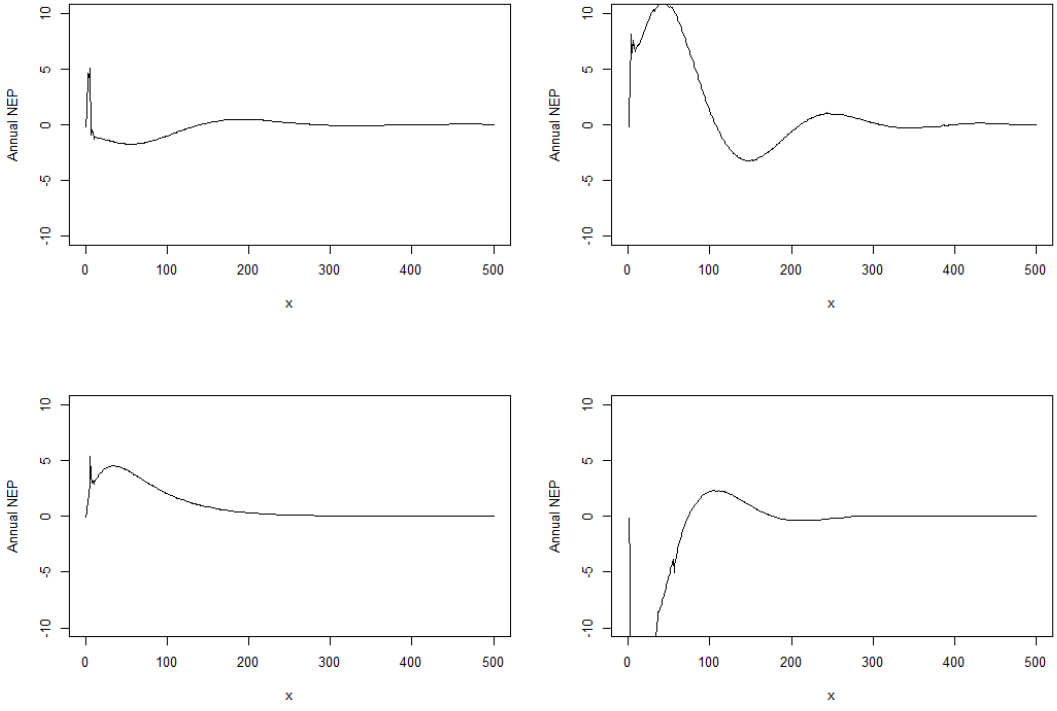
210 Fig. 1. Algorithms and procedures of the new spin-up method

211

212

213

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018



214

215 Fig. 2. The time for NEP (g C $yr^{-1}m^{-2}$) reached a steady state with the original spin-up method at

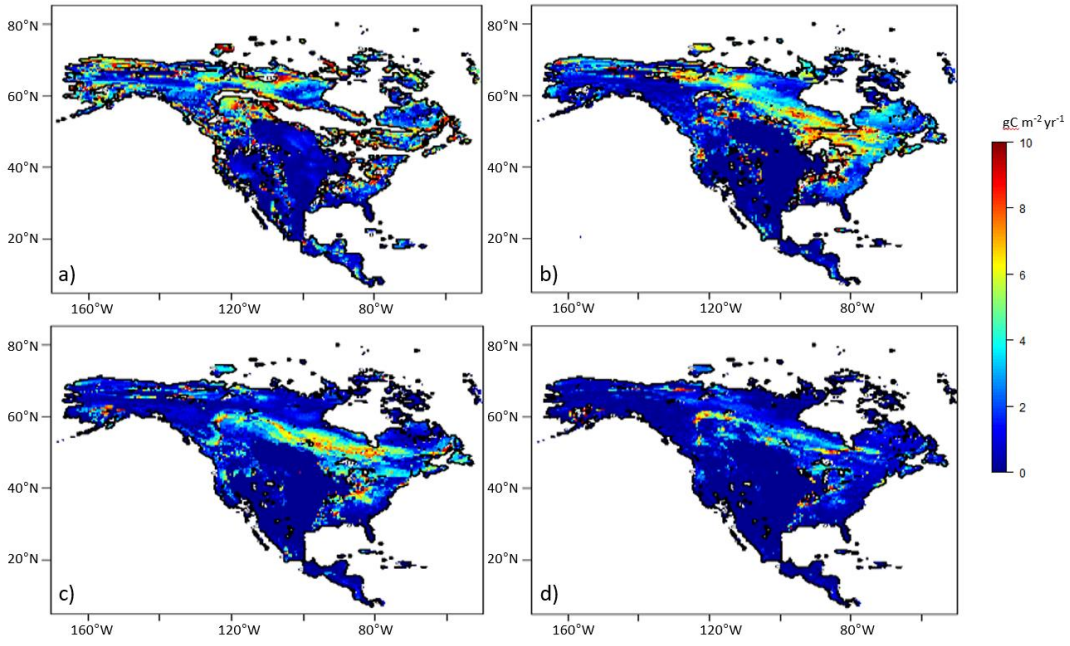
216 Harvard forest site. x represents model simulation years.

217

218

219

Biogeosciences Discuss., https://doi.org/10.5194/bg-2018-98
Manuscript under review for journal Biogeosciences
Discussion started: 12 March 2018



220

221 Fig. 3. The spin-up time to reach the steady state of NEP (g C m^{-2} yr^{-1}) with the original spin-
222 method: In 50, 100, 150, and 200 years, 63%, 89%, 93%, and 98% grids will reach their steady
223 states, respectively.

224

References:

Bey, I., Jacob, D. J., Yantosca, R. M., Logan, J. A., Field, B. D., Fiore, A. M., ... & Schultz, M. G. (2001). Global modeling of tropospheric chemistry with assimilated meteorology: Model description and evaluation. Journal of Geophysical Research: Atmospheres, 106(D19), 23073-23095.

Comins, H. N. (1997). Analysis of nutrient-cycling dynamics, for predicting sustainability and CO 2-response of nutrient-limited forest ecosystems. Ecological modelling, 99(1), 51-69.

Dickinson, R. E., Shaikh, M., Bryant, R., & Graumlich, L. (1998). Interactive canopies for a climate model. Journal of Climate, 11(11), 2823-2836.

Henze, D. K., & Seinfeld, J. H. (2006). Development of the adjoint of GEOS-Chem. Atmospheric Chemistry and Physics Discussions, 6(5), 10591-10648.

Johns, T. C., Carnell, R. E., Crossley, J. F., Gregory, J. M., Mitchell, J. F., Senior, C. A., ... & Wood, R. A. (1997). The second Hadley Centre coupled ocean-atmosphere GCM: model description, spinup and validation. Climate dynamics, 13(2), 103-134.

King, D. A. (1995). Equilibrium analysis of a decomposition and yield model applied to Pinus radiata plantations on sites of contrasting fertility. Ecological modelling, 83(3), 349-358.

Kwon, E. Y., & Primeau, F. (2006). Optimization and sensitivity study of a biogeochemistry ocean model using an implicit solver and in situ phosphate data. Global biogeochemical cycles, 20(4).

McGuire, A. D., Melillo, J. M., Joyce, L. A., Kicklighter, D. W., Grace, A. L., Moore, B. I. I. I., & Vorosmarty, C. J. (1992). Interactions between carbon and nitrogen dynamics in estimating

net primary productivity for potential vegetation in North America. Global Biogeochemical Cycles, 6(2), 101-124.

Michalakes, J., & Vachharajani, M. (2008). GPU acceleration of numerical weather prediction. Parallel Processing Letters, 18(04), 531-548.

Nvidia, C. (2007). NVIDIA CUDA Compute Unified Device Architecture Programming Guide. NVIDIA Corporation.

Thornton, P. E., & Rosenbloom, N. A. (2005). Ecosystem model spin-up: estimating steady state conditions in a coupled terrestrial carbon and nitrogen cycle model. Ecolo

Xia, J. Y., Luo, Y. Q., Wang, Y. P., Weng, E. S., & Hararuk, O. (2012). A semi-analytical solution to accelerate spin-up of a coupled carbon and nitrogen land model to steady state. Geoscientific Model Development, 5(5), 1259-1271.

Xiu, D., & Karniadakis, G. E. (2002). The Wiener--Askey polynomial chaos for stochastic differential equations. SIAM journal on scientific computing, 24(2), 619-644.

Xiu, D., & Hesthaven, J. S. (2005). High-order collocation methods for differential equations with random inputs. SIAM Journal on Scientific Computing, 27(3), 1118-1139.

Zhu, Q., Zhuang, Q., Henze, D., Bowman, K., Chen, M., Liu, Y., ... & Oechel, W. (2014). Constraining terrestrial ecosystem CO 2 fluxes by integrating models of biogeochemistry and atmospheric transport and data of surface carbon fluxes and atmospheric CO 2 concentrations. Atmospheric Chemistry and Physics Discussions, 14(16), 22587-22638.

Zhuang, Q., McGuire, A. D., Melillo, J. M., Clein, J. S., Dargaville, R. J., Kicklighter, D. W., ... & Hobbie, J. E. (2003). Carbon cycling in extratropical terrestrial ecosystems of the Northern

Hemisphere during the 20th century: a modeling analysis of the influences of soil thermal dynamics. Tellus B, 55(3), 751-776.

Zhuang, Q., He, J., Lu, Y., Ji, L., Xiao, J., & Luo, T. (2010). Carbon dynamics of terrestrial ecosystems on the Tibetan Plateau during the 20th century: an analysis with a process-based biogeochemical model. Global Ecology and Biogeography, 19(5), 649-662.