Response letter

Thanks for your constructive comments. Below we detail how we revised the manuscript following your suggestions.

(1) clarify the equations and method adopting the half time step approach

Response: In this revision, we went through all equations to ensure they are correct. For instance, we change x to $\vec{x}$. *We changed g(x) to* $g(\vec{x},t)$ *to make consistent in equations 9 and 10. In addition, we added the following sentence to clarify the half time step approach: "Here ½ refers to the half time step in the middle of a month, at which values of J are calculated as the mean value at time steps k and k-1. x0 refers to the initial pool size.".*

(2) underscore how the use of TEM may differ from a similar application with more complex models;

Response: In this revision, we added some discussion on the implementation of this new spin-up method in TEM vs. in other models with more state variables, to underscore the differences implemented in TEM and other models: "The TEM model has a relatively small set of state variables for carbon and nitrogen. The version we used is TEM 5.0, which has only five state variables (Zhuang et al., 2003). Thus, the linearization process is relatively easy and the matrix size is relatively small, consequently, the computing is not a burden. To accelerate the spin-up for multiple soil carbon pool models with relatively simple and linear decomposition processes, implementing our method shall be still relatively easy, but will take a great amount of computing time to equilibrate. For models such as CLM, multiple methods have been tested to accelerate their spin-up process (e.g., Fang et al., 2015), the direct analytical solution method introduced in this study might be time-consuming to achieve.".

(3) include a discussion, as in the response to R2, about the spin-up time achieved for TEM and how it relates to what would be achieved for applications to more complex models such as CASA and Century;

Response: See our response (2) above. In addition, we added a few sentences to discuss how our new method could be applicable for other models in the Summary section: "We consider our method is a general approach to accelerate the spin-up process for process-based biogeochemistry models. As long as the governing equations of the models can be formulated as the form in eq. (9), the algorithm could be adopted accordingly.".

(4) clarify the terminology for LU;

Response: We added the full name for LU. The definition of LU is Lower and Upper operation.

(5) re-iterate that the application seeks an annual steady state for a cyclo-stationary, monthly time step model rather than a monthly steady state

Response: We made the statement clear, i.e., the spin-up method is targeting an annual steady state for a cyclo-stationary, rather than a monthly steady state, by adding "While our new approach runs the model at monthly time step with the cyclic boundary conditions for state variables x, it still targets a steady state for the ecosystem at annual time step instead of monthly time step.".

(6) additional details on applications at other sites listed in Table 1, and the proposed revisions to Table 2

Response: In this revision, we included spin-up performance for all 7 study sites with different spin-up methods as requested. These seven sites represent the key plant functional types in North America. The site information was documented in Table 1. Based on Table 2, we added a few sentences to describe the performance of the new method in comparison with other methods: "For all seven test sites, the original spin-up method in TEM takes 204-564 years (1.1-2.5 seconds of computing time) to reach the steady state at different sites. In contrast, our new method only takes 0.3-0.6 seconds, while the semi-analytical method (Xia et al., 2012) will need 0.5-0.9 seconds to reach the steady state at different sites (Table 2).".

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

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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 by finding the exact solution of a linearized system representing cyclo-stationary state of a model 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 be used for future quantification of carbon dynamics at fine spatial and temporal scales.

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 in some extreme cases. 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. However, Lardy et al (2011) and Martin et al (2007) have implemented their spin-up methods for a linear problem of soil carbon dynamics including their seasonal cycles.

Here we developed a -method to accelerate the spin-up process in a non-linear model. 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:

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

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

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

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

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

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:

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

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

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

For detailed GPP definition, see Zhuang et al. (2003). 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:

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

Where $\vec{x}$ ~~*~~ is a vector of state variables (e.g., C_V); $\vec{h}(t)$ ~~$\vec{h}$~~ is the vector of carbon/nitrogen input from the atmosphere, independent on $\vec{x}$; $g(\vec{x},t)$ ~~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:

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

where g represents $g(\vec{x},t)$. $\vec{x}_n$ represents each of state variables in the TEM. The numerical discretization of equation (9) is:

$$x_{i,k} - x_{i,k-1} = \tau \cdot J_{k-\frac{1}{2}} \cdot x_{i,k-1} + \tau\left(g(x_0,k-1) - J_{k-\frac{1}{2}} \cdot x_{0,k-1} + h_{k-1}\right) \quad \text{.....(12)}$$

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

Where τ is time step (month), x_k is the pool size at time k, $J_{k-\frac{1}{2}}$ is a Jacobian matrix at time step $k-\frac{1}{2}$. Here ½ refers the half timestep in the middle of a month, at which values of J are calculated as the mean value at time steps k and k-1. $x_{i,0}$ refers to the initial pool x_i size.

~~are calculated as the mean value at time steps k and k+1. x_0 refers to the initial pool size.~~

We introduce:

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

The eq. (12) can then be written as:

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

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

Where $J_{k-\frac{1}{2}}$ is a Jacobian matrix at the time step $k-\frac{1}{2}$. 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 further written as:

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

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

Then Eq. (13) will become:

$$-C_1 \cdot x_T + B_1 \cdot x_1 = y_1 \text{.....(15}a\text{)}$$

Thus eq. (15) and (15a) become a formulation of a linear problem with T unknown vectors x_k, which can be solved using LU (lower and upper) decomposition or Gaussian elimination (Martin et al., 2007). Xia et al (2012, see Eq. 4) and Kwon and Primeau (2006) also had linear equations for a steady state, but conduct the model simulation at annual time step. Going for annual average form reduces the size of the ~~problem, and~~problem and prevents Xia et al (2012) from obtaining the exact solution of the problem including seasonal cycle (see their Eq. 15, 15a). While our new approach runs the model at monthly time step with the cyclic boundary conitions for state variables x, it still targets a steady state for the ecosystem at annual time step instead of monthly time step.

2.3 Numerical implementation

Eq. (15a) is explicitly expressed as:

$$\begin{pmatrix} B & 0 & 0 & \dots & 0 & 0 & 0 & -C \\ -C & B & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & -C & B & \dots & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & -C & B & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & -C & B & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & -C & B \end{pmatrix} \times \begin{pmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ . \\ . \\ x_T \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ . \\ . \\ . \\ . \\ . \\ y_T \end{pmatrix}$$

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

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

We apply the Gaussian elimination to upper block that reduces M to a lower triangular form (Figure 1). The elimination process is applied from right to left in the top row of M involving 2x2 blocks of matrices B_k, C_k, D and D^1.

~~B, C, D and D^1.~~

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

The resulting matrix is lower diagonal:

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

The eq. (16) is thus reduced to form $M'x = Y'$, where M' is lower diagonal, and solution of eq. (15a and 16) will be readily obtained for x.

2.4 Algorithm implementation for TEM

In the original TEM, carbon fluxes can be defined as:

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

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

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

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 C_V and temperature (K_T). Here we revised MR calculation:

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

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 (for TEM n=5) 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 plant functional types (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. ~~3.~~ Results and Discussion

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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). In contrast, 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. The new method performs similarly for the rest of six sites.

For all seven test sites, the original spin-up method in TEM takes 204-564 years (1.1-2.5 seconds of computing time) to reach the steady state at different sites. In contrast, our new method only takes 0.3-0.6 seconds, while the semi-analytical method (Xia et al., 2012) will need 0.5-0.9 seconds to reach the steady state at different sites (Table 2). Compared to the original spin-up method, the new method is not only faster, but also computationally stable.

~~For all seven test sites, it takes on average 0.6 seconds using the 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.~~

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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, 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:

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

Where P(t) is a vector of pools in TEM (e.g., C_V and C_S). 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).

The TEM model has a relatively small set of state variables for carbon and nitrogen. The version we used is TEM 5.0, which has only five state variables (Zhuang et al., 2003). Thus, the linearization process is relatively easy and the matrix size is relatively small, consequently, the computing is not a burden. To accelerate the spin-up for multiple soil carbon pool models with relatively simple and linear decomposition processes, implementing our method shall be still relatively easy, but will take a great amount of computing time to equilibrate. For models such as CLM, multiple methods have been tested to accelerate their spin-up process (e.g., Fang et al., 2015), the direct analytical solution method introduced in this study might be time-consuming to achieve.

~~To accelerate the spin-up for multiple soil carbon pool models with relatively simple and linear decomposition processes, implementing our method shall be relatively easy, but will take a great amount of computing time to equilibrate. For models such as CLM, multiple methods have been tested to accelerate their spin-up process (e.g., Fang et al., 2015), the direct analytical solution method might be time-consuming to achieve.~~

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

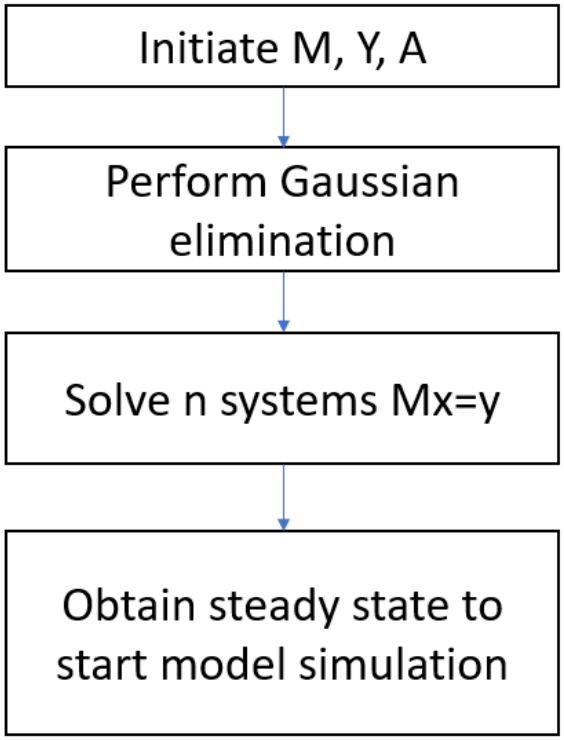
using the traditional method. For regional simulations in North America, average spin-up time saving is 85% for either daily or monthly version of TEM. We consider our method is a general approach to accelerate the spin-up process for process-based biogeochemistry models. As long as the governing equations of the models can be formulated as the form in eq. (9), the algorithm could be adopted accordingly. Our method will significantly help future carbon dynamics quantification with biogeochemistry models at fine spatial and temporal scales.

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]

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


Initiate M, Y, A
Perform Gaussian elimination
Solve n systems Mx=y
Obtain steady state to start model simulation

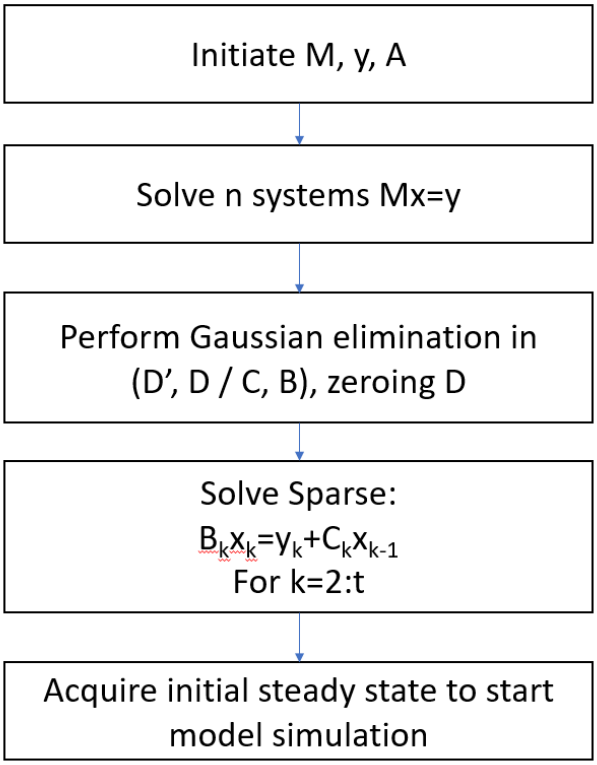


Fig. 1. Algorithms and procedures of the new spin-up method

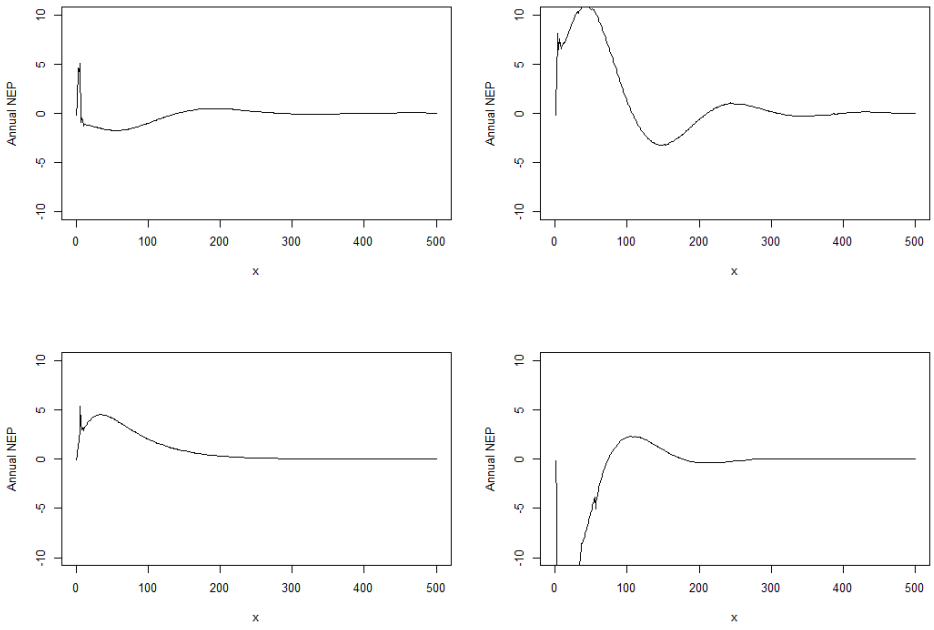


Fig. 2. The time for NEP (g C $yr^{-1}m^{-2}$) reached a steady state with the original spin-up method at Harvard forest site. x represents model simulation years.

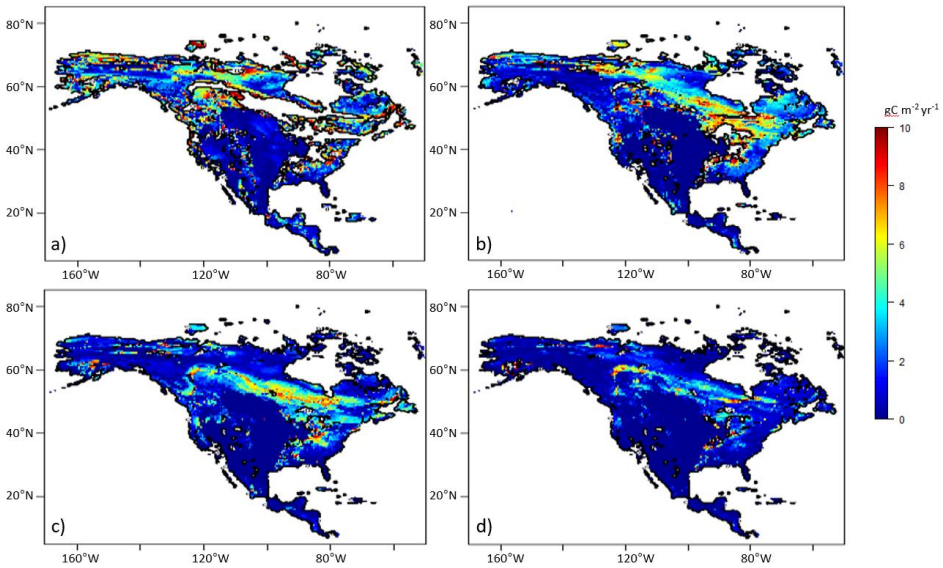


Fig. 3. Simulated NEP (g C m^{-2} yr^{-1}) with the original spin-method after different spin-up years of (a) 50, (b) 100, (c) 150, and (d) 200 years, respectively. After these spin-up years, 63%, 89%, 93%, and 98% grids will reach their steady states, respectively.

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