Overall response:

While we appreciate the reviewer's time to review our study, we believe the reviewer has mis-construed significant parts of our arguments and results. We address all the comments below, but note in particular that the reviewer's repeated contention that calibration can make a numerically inconsistent model useful for projecting carbon-climate feedbacks highlights why we think out study is important for the modeling community. We make the point in our paper that, at the most basic level, models require that the numerical encoding is consistent with their analytical formulations. The practice of ensuring this consistency has been standard in other branches of earth system modeling, including atmospheric physics (e.g. Phillips, 1956; Arakawa, 1965; Wan et al., 2016), atmospheric chemistry (Sandu, 2001; Nguyen et al., 2009; Wan et al., 2013), hydrology (Tang et al., 2015) and marine biogeochemistry (Broekhuizen et al., 2008); land biogeochemical modeling should be no exception. Consistent and robust numerical encoding can help ensure that new mechanisms and processes are added for the right reasons, and can remove the false security generated by calibration of structurally uncertain biogeochemical models. Further, our study shows that numerically inconsistent models can result in very misleading predictions of how land ecosystems respond to increasing atmospheric CO_2. If the reviewer's opinions on the appropriate use of calibration are widespread in the modeling community (which we believe is the case), we contend that our paper is very relevant and important, in that it dispels those notions and proposes constructive remedies. With the spirit to raise sufficient awareness of these important issues, we carefully address the reviewer's comments point by point below.

Comment 1: I find this study intriguing. There has been a debate about the definition of nutrient limitation (see Davidson and Howarth 2007; Elser et al. 2007 and many more), different representations of nitrogen limitation in numerical models simply reflect those diverging views. What implications of different numerical representations of nitrogen limitation will have on the projected land carbon sink is an important question, and needs a careful study. This study found significant discrepancies in the projected land sinks by ALM using different representations of nitrogen limitation. The results are interesting. However little explanation has been given to why they are different. I also found some results quite intriguing. The other issue identified in this study is double counting of nitrogen limitation. This has been pointed out by others before (Downing et al. 1999; Agren et al. 2012 for example). The issue of double-counting is less prevalent, as several global nutrient models, OCN, CABLE and GFDL land models do not use CLM-like approach, i.e. reducing GPP when nitrogen demand by plants is higher than available N. OCN and CABLE will vary allocation and tissue chemistry, which will affect GPP, canopy LAI from next time step on.

Response: We thank the reviewer for taking his/her time to review our manuscript and we appreciate his/her positive comments. At the broadest level, there are two aspects associated with how nitrogen limitation is implemented in models: the analytical formulation of the mechanisms and the numerical implementation of those mechanisms. The aspect that the reviewer mentioned above refers to the first (the analytical formulation of nitrogen limitation controls, or growth-controlling in the term recommend by Kovarova-Kovar and Egli (1998)), and the CLM-like formulation is just one of the many formulations used. We focused our study on the second (numerical aspects of the CLM-like implementation), and demonstrated that an inconsistent numerical implementation (Mineral Nitrogen based Limitation (MNL) or Net Uptake based Limitation (NUL)) of the CLM-like formulation resulted in large differences in simulated cumulative land carbon fluxes when compared to that simulated from a consistent numerical implementation (Proportional Nitrogen Limitation (PNL)). Throughout the revised text, we clarify these points.

Second, as for explanations as to how the differences arise, we refer the reviewer to section 4.1 in our first submission and also the revised text, where we applied single-point simulations to investigate these differences. The explanation is quite simple: when both nitrate and ammonium are explicitly competed, the PNL approach resulted in higher nitrification rates (as compared to MNL or NUL), as it allows the newly released ammonia from decomposition to be nitrified, which further enhances nitrogen losses through denitrification and hydrological losses. When this difference is convolved with the high CN ratio of plants, the differences are amplified in the carbon dynamics. In the revised text, we enhance our discussion on how these large differences arise (see section 4.1 and 4.2).

Third, we carefully checked the papers on double counting of nitrogen limitation brought up by the reviewer. We found the "double counting" referred to in these papers is a different concept from the one described in our submitted paper, and that Downing et al. (1999) and Agren et al. (2012) were each taking different viewpoints on different subjects. Downing et al. (1999) were discussing how to experimentally estimate the limitation effect in a phytoplankton fertilization experiment, and concluded that bulk cell biomass rather than bulk growth rate should be used for calculating the nutrient limitation effect. Agren et al. (2012) were analyzing how nutrient co-limitation should be analytically formulated for individual plants. We highlighted these differences in our revised text to ensure other readers will not have this confusion (P6, L7-8).

In contrast, our statement of double counting is that there is a local limitation imposed on each individual through the analytical formulations (using law of the minimum), whereas the ultimate limitation is coming from the interactions of all competitors in the system. So if the law of the minimum is used for modeling nutrient limitation, it should be imposed at the system level, which will result in consistent constraints on individuals in the network. None of the papers referred by the reviewers have pointed out this issue. For this reason, as long as (1) some form of law of the minimum is implemented in a model and (2) the nutrient levels will reach some negative value (if fluxes are not corrected) at some simulation step, double counting will always occur. Given that the law of the minimum is applied to individuals without simultaneous consideration of the overall system constraints in all BGC models we are aware of, this issue is not unique to the CLM-like approach.

Comment 2: The title: Given several caveats of this study, the title is misleading. The "large" uncertainty can result from lack of adequate model calibration, initialization and so on. Even this uncertainty is large for ALM, and may not be for other models.
Response: To make our assertion more conservative, we revised the title as "Potentially large uncertainty in ecosystem carbon dynamics resulting from ambiguous numerical coupling of carbon and nitrogen biogeochemistry: A demonstration with the ACME land model."

Comment 3: P1, L8. “Abstract” “Most earth system models (ESM): : :” . That is not true, essentially only one model includes N cycle among all AR5 ESMs.
Response: Our description is accurate, since, subsequent to the CMIP5 exercise, most models are incorporating the N cycle, and even P cycle, in their development. Some published references are CABEL (Wang et al., 2010) that is coupled to CSIRO Mk3L climate system model, JSBACH (Goll et al., 2012), UVic ESCM (Wania et al., 2012), CESM, and ACME (which we refer to in this study).

Comment 4: P1, L15-16. Comparing the divergence here that is supposed to be caused by different approaches of N limitation with the divergence among mostly carbon-only model is not appropriate.
Respond: Since we are comparing different uncertainty sources, we believe this comparison is appropriate as has been shown in previous studies (Clein et al., 2007; Huntingford et al., 2013; Tang and Zhuang, 2008). Further, the importance of developing better models of nitrogen dynamics is clear if the divergence from models with nitrogen dynamics is comparable to or larger than that of the carbon only model.

Comment 5: P1, L20-21. “..significant sensitivity of model prediction to initial conditions: : :”. For each representation of N limitation, how different are the equilibrium pool sizes and fluxes? If you did not spin each representation to steady state separately, the issue here may be related to initialization and calibration (GPP being too high in this study), not initial values.
Response: First, we have spun up all simulations separately, and the results indicate that their differences are small (for a few example variables, see Figures X1-X4 at the end of this response, where the spatial distribution of vegetation carbon, vegetation nitrogen, soil carbon and soil nitrogen were found coherent among different models). These small differences are also consistent with the small differences we show in Figure 1 for models excluding PNLIC.

Second, we do not think the calibration issue is relevant here, as we are using the same parameter values of the default model, and the reported variables in the 1990s are very similar between our new simulations and the default model. We do note that PNLIC is an outlier from the other simulations. This significant difference results from our purposeful running of the PNL model using initial conditions from NUL. In this way, as we explained, PNLIC is used to demonstrate the possible model misuse when the numerical implementation of the model is not well acknowledged to the user. In particular, the rationale behind this numerical experiment is that if we assume two modelers are given the same set of equations to solve, they will obtain very similar results, such that the initial conditions between these two models can be legitimately switched. However, our survey and evaluation in this study (see also Tang and Riley, 2016) indicates that this may not be the case. We also highlight that many modeling papers have not explicitly described their model's numerical details, which may lead to non-reproducible predictions if one tries to recreate the model from scratch and use it for the same type of model simulations.

Comment 6: P2, L1-11. I do not really appreciate the rationale for classifying the "errors" identified in this study into a combination of type I and II. The "errors" simply result from model structure differences. To some extent, errors in numerical implementation can be part of model structure error. I found the identification of four-stages of model design unhelpful. The authors did not follow each of these four stages through in this study, as they did not calibrate the different representations. If they have calibrated different representation using same datasets, the divergence among different representations may be much smaller, and the conclusions from this study may not be accurate any more. Given this caveat, results from this study are better suited for a technical note for ALM model development community.

Response: While we agree that classifying the "errors" identified in this study into a combination of type I and II may be a personal preference, we do not agree with the loose definition of model structural differences advocated by the reviewer. If considering the "model structure" as any difference in the model's encoding (e.g., numerical methods), then if the model parameterization is hardwired in the model (as many models do), the model parameterization uncertainty can be regarded as model structural differences as well. We therefore, in the spirit of rigorous model development and application, suggest that the four stages of model design are necessary and helpful, and are more logical than over generalizing the concept of structural uncertainty. In a nutshell, model development and application is one manifestation of applied mathematics, which involves analytical formulation, numerical discretization, parameterization, and application, which are accordant with the four stages we classified. Given this argument, the classification of our identified errors into a combination of type I and II is logical and appropriate.

Further, we think the reviewer has exaggerated the effect and usefulness of model calibration. In all types of modeling work that involve the solution of differential equations, the first step should be to solve the equation in a numerically consistent way. This is why Lax and Richmyer (1956) proposed Lax's equivalence theorem on numerical consistency, which has been the golden standard for solving differential equations (e.g. Smith, 1985). When the model is not solved in a numerically consistent way, calibration is a waste of resources.

The problem we identified here is not unique to ALM (as we argued previously and elaborate further here). On the contrary, the problem of mis-coupling of various modeling components (or physical processes) has been identified in the modeling of atmospheric physics (Wan et al., 2016), atmospheric chemistry (Sanddu 2001; Nguyen et al., 2009; Wan et al., 2013), hydrology (Tang et al., 2015), marine biogeochemistry (Broekhuizen et al., 2008), combustion systems (Gou et al., 2009), and many others. We have added this argument and citations to the revised manuscript. There are even workshops specifically discussing this type of problem (e.g., Workshop on Physics Dynamics Coupling (http://events.pnnl.gov/default.aspx?topic=Physics_Dynamics_Coupling_in_Weather_and_Climate_Models). Therefore, misinterpreting that our results are unique to ALM will further hide such issues in land biogeochemical modeling, rather than to help resolving the large uncertainty in current and maybe future predictions of carbon-climate feedbacks.

Comment 7: P2, L28-29. Here you stated: "numerical implementation of a given formulation" is the focus of this study. What are your given formulation? Equations (3), (6), (7) and (8) are mathematically different? I think that your study is about different implementations of nutrient limitation effect, not numerical implementation of the same equations.

Response: The formulation we are referring to is the land biogeochemical model of CLM4.5 and ALMv0, which is documented very thoroughly in the technical note (Oleson et al., 2013). Since equations (6), (7), and (8) attempt to numerically approximate the same equation, i.e. equation (2), they are therefore different numerical implementations of the same equation.

Comment 8: P3, L14-15. This is not how nutrient limitation is defined in several others global land models. Nutrient limitation can occur even if the nutrient demand is met by uptake. For example, in a fast-growing plantation, the plants will try to increase its LAI first, then its leaf N:C ratio, or both. If LAI increases first, the leaf N:C ratio is low, the canopy photosynthesis is considered to be N limited because adding N fertilizer will increase canopy photosynthesis by increasing leaf N:C ratio, or canopy LAI or both. The CLM alike approach is not adopted by most other global land models. You should not generalize it to other models here.

Response: We clarified in our original submission (P2, L26-29) that there are two aspects of nutrient limitation: one is the analytical formulation and the other is the numerical implementation. The analytical formulation (e.g., that implemented in CLM4.5) includes all aspects that the reviewer is mentioning here. The numerical implementation specifically refers to the study we describe here. We have revised the paper to further clarify this issue (by adding appropriate references and more descriptions, P2 L29-33, P3:L1-L12). Also, we note a few other models have also adopted the CLM/ALM-like approach, e.g. Biome-BGC (Thornton et al., 2002), BiomeBGC MuSo (Hidy and Barcza, 2014), and JSBACH (Parida, 2011; Goll et al., 2012). So we are not over generalizing our results as inferred by the reviewer.

Comment 9: P3, L25 "..substrate production is independent of consumption, a situation that occurs exactly in the CENTURY-like models". That is incorrect. If true, progressive nitrogen limitation will not happen in CENTURY-like models, such as G'DAY.

Response: We mentioned that there are two aspects of nitrogen limitation: the formulation aspect is referred throughout the reviewer's comments, whereas we are only discussing the numerical aspects. Therefore, as long as nitrogen dynamics are coupled with carbon dynamics, and nitrogen availability is insufficient to support potential assimilation, progressive nitrogen limitation will always occur. However, what we meant at P3, L25 is that the nitrogen mineralization of some SOM (soil organic matter) pools is not an explicit function of nitrogen uptake from other SOM pools. This dynamic occurs in Century-like models because the different SOM pools decay independently, such that a nitrogen mineralizing pool experiences no nitrogen stress from the concurrently nitrogen immobilizing SOM pools. To avoid this misunderstanding, we add clarifying explanation in our revision (P4: L16-18).

Comment 10: P4, L13-15. But S is a function of N mineralization rate as stated in eqn (1). I disagree with your interpretation here.
Response: We note that (3) is using the nitrogen pool from the current time step, so our explanation is correct. Also we stated when introducing equation (2) that we are using the forward Euler scheme for model integration. Therefore, this misunderstanding should not arise.

Comment 11: P5. L17. "applying the flux adjustment only to Fs,uptake". By authors' argument, will this also constitute a double–counting of nutrient limitation?
Response: If this flux adjustment is coupled with an explicit use of law of the minimum, then double counting of nutrient limitation can occur. We avoided it in our study by using the scheme described in Tang and Riley (2016).

Comment 12: P5, Write eqn (7) using notation of t, t+1, or implicit form.
Response: We decide to keep it as is in order to avoid further complication and confusion because we stated explicitly that we are using the forward Euler scheme when introducing equation (2).

Comment 13: P5, eqn (6) and (7), I really not see much differences between these two equations in practice. One can also argue that both N input and available mineral soil N

are available for plant uptake in the NUL formulation.
Response: The difference occurs in the numerical implementation when the limitation strength predicted by equation (6) is stronger than that by equation (7) under the same conditions. We have provided our mathematical proof of this situation in the originally submitted (and also the revised) supplemental material.

Comment 14: P6, Eqn (8). This is an incorrect interpretation of eqn (C12) of Wang et al. (2010). Wang et al. (2010) did not represent N uptake by decomposers explicitly.
Response: We did not understand the reviewer's meaning here. Nevertheless, in Wang et al.'s equation (C12), the model imposes nitrogen limitation based on net unlimited N mineralization, which is used exactly in equation (8) of our submitted paper.

Comment 15: P6, L18-25. After all, you treated all three approaches as being valid, which contradicts to your earlier arguments that MNL counts for nutrient limitation twice, and NUL requiring flux adjustment that also constitutes double counting of nutrient limitation based on authors' argument.
Response: We believe this is another misunderstanding of our study. The double counting has no direct connection to MNL, NUL, or PNL. Rather the double counting results from first applying law of the minimum on individual consumers, and then rectifying the nutrient fluxes a second time if the nutrient stock would become negative without such rectification. See our response to comment 1 for further discussions.

Comment 16: P6. "ambiguous numerical implementation"? Numerical implementation is not ambiguous, but its interpretation is.
Response: We acknowledge that numerical implementation may also be a mathematical manifestation of ambiguous interpretation; when the interpretation is ambiguous, so is the numerical implementation, and vice versa.

Comment 17: P7, L23-30. You removed the down-regulation of GPP. That is theoretically better. However you did not re-calibrate your GPP, therefore your estimated plant N demand is excessive, and may not be met at available soil N. This could be the cause for the oscillatory responses shown in Figure 2. At a given time step, if available soil N plus mineralized N is less than the N demand by plant and microbes, you have to use flexible C:N ratio approach, independent of whichever numerical representations. Here it is important to state whether you have flexible C:N ratios for all pools, and what are the ranges of C:N ratios? What do you do when demand by plants and microbes is higher than available soil mineral N and mineralized N at a given time step? And how different numerical representation deal with this issue while maintaining mass conservation.

Response: First, the oscillatory response in Figure 2 resulted from the cycling of climate forcing data (we clarified this in the revision by stating it clearly in the figure captions), and has nothing to do with the removal of GPP down-regulation. In the revised text, we state clearly that the version of the model used here applies fixed C:N ratios and that testing with flexible C:N is underway, and will be reported elsewhere. Further, in the models we are comparing, all use the same model parameters, as they are arguably solving the same set of model equations. Therefore, the calibration is not a relevant issue here. Finally, we did check that the revised models are behaving similarly as the default model in the historical period (also see response to comment 5), and have added description to this effect in the revised manuscript.

Comment 18: P7, L25. If you simply remove this down-regulation without tuning your model properly, you will have very high N demand in your model, which likely causes much numerical issues in your integration, such as mass conservation. What you should do is to reduce the potential GPP calculated by your model by calibration.

Response: As we argued previously, the calibration is not a relevant issue in this study, given that our model results for the contemporary period are quite close to the default CLM4.5 and ALMv0, which have been reviewed, publically released, and applied in many studies. Also, the mass conservation issue raised by the reviewer has been very carefully addressed, and in fact, if the masses of carbon, nitrogen, and water are not conserved, our model will stop and issue an error message to that effect.

Comment 19: P8. L1-9. CENTURY-like models do not allow any preference by plants or soil microbes between NH4 and NO3. This is not a CENTRY-thing.
Response: We revised the language to make the statement less specific to CENTURY-like models.

Comment 20: P8, L10-22. When using each of five different numerical implementations, did you spin the model to steady state for each of them? I do not think that PNLIC is a valid one.
Response: Yes, we did careful spinup for all simulations. PNLIC is an intentional simulation with PNL using initial conditions from NUL, which reflects the incompatibility of the two models. This simulation is one example to demonstrate the potential danger if the numerical implementation is not acknowledged to the user. See our response to comment 5 for further discussions.

Comment 21: P8, L18 ".. finally applied nitrogen limitation to microbes and plants a second time". How? Give more details here. What is the justification of applying nitrogen limitation twice?
Response: We explained in the text that because this is the only way to prevent the model from crashing (through negative nitrogen or oxygen concentrations). This approach is equivalent to the projector-corrector methods, where the first step is making a prediction, and the second step is a correction to impose the actual nitrogen limitation through linear downregulation.

Comment 22: P9, Section 2.2. How can you use the Qian et al's data of 1848 to 1972 to generate the forcings from 1850 to 2005 for ALM? Here you stated that all model simulations span to steady state at 1850. How different are the steady state pools and fluxes among different numerical representations at 1850? Why diagnostic atmospheric CO2 concentrations (L4)? How different are your diagnostic CO2 concentrations from the observed CO2 concentrations from 1850 to 2000? Did you include land use change in your simulated land carbon dynamics (L8)?
Response: Yes we spun up all models. The diagnostic CO_2 concentrations means using

observed atmospheric CO_2 concentrations. We included land use change using the standard approach in CLM4.5, and since all simulations were run with the same protocol, the details of land use change are not relevant here. In addition, this practice is standard in applying CLM or ALM.

Comment 23: P9, Figure 1. I find the results very puzzling. Given that NPP is similar among six different approaches, soil C is also quite similar except that the red curve is generally higher than others across different latitudes. Can the large differences in the simulated NEE be explained by the differences in the simulated heterotrophic respiration among five different approaches? Does each of the five approaches conserve mass of C and N? We need this evidence to be convinced that the numerical implementation of all five approaches are accurate. I do not see any relevance of showing latent heat flux here. Also the canopy LAI in the tropics and high latitudes (about 60degree North) is unrealistically high (>6). As a result, your N demand is also unrealistically high.
Response: By design, our models maintain rigorous mass balance for carbon, nitrogen, and water. The differences between the models (excluding PNLIC) are within the range of uncertainties as reported in other studies. We are aware that CLM does not simulate reliable LAI because its poor representations of the carbon and nutrient allometry and stoichiometry. These issues are under improvement and results will be reported elsewhere. However, as we explained above and in the revised manuscript, these issues will not change the conclusion of our study.

Comment 24: I suspect that the divergent results as shown in Figure 1 may be complicated by the lack of mass conservation for some approaches, therefore it is difficult to separate the effect of not conserving mass from different representations of N limitation on the simulated variables. I think that the authors incorrectly attribute all the differences shown in Figure 1 to the representation of N limitation (also see my comment 9).
Response: As we explained, our models have rigorous mass balance checks for carbon, nitrogen, and water. Otherwise, the model will stop and no simulations could be done.

Comment 25: Among the five approaches, I think that PNLIC being invalid and PNLO being a different issue. I suggest that authors remove the results from those two approaches. The presentation of the results, particularly in Figures 1 and 2 are very difficult to distinguish.
Response: With all our explanations above, we decide to keep PNLIC and PNLO in our results. Also, the other reviewer has no complaints about Figures 1 and 2.

Comment 26: Figure 1. All six approaches simulated very similar GPP, NPP, soil carbon, but the cumulated NEE by PNLIC is 50 times greater than most other approaches? Where does this huge amount of carbon come from? Please show changes of global carbon pools (vegetation, soil, litter) as well as fluxes in this Figure. Has mass been conserved in all approaches. If not, then the results are not valid.
Response: Once again, we addressed the reviewer's concern regarding mass balance in previous comments. The difference is from shifted partitioning between nitrogen losses and nitrogen uptake: when combined with the usual high CN ratio of vegetation and SOM pools, the small differences in nitrogen turns into large differences in carbon. We have provided some of this extra information in the supplemental material in our first submission, and we enhanced relevant explanations in both the revised text and supplemental material.

Comment 27: P10. Section 3.2 and Figure 2. Even being averaged over such broad regions (north temperate, tropics and artic), the results still show some periodic oscillation. This needs some detailed explanation. How can we have any confidence in any of the results if masses of C and N are not conserved? Why the changes in vegetation and soil carbon (shown in a2 and a3) do not add up to total carbon change (a1)? Similarly for other two regions as well.
Response: As described above, the periodic oscillation results from the recycling of climate forcing. We further clarified this in our revised manuscript. Once again, the reviewer's questioning on mass balance has been addressed: the models all conserve mass.

Comment 28: I do not know how much of the results are applicable to other models. I think that the authors oversell their results a bit by using very high GPP, therefore high N demand, which differs from other global models. If a more realistic GPP, therefore N demand are used, will the differences among different approaches still be so large?
Response: To the contrary, we believe our results are highly valuable because they are made on the generic point of ambiguous numerical implementation of nutrient effects on the carbon cycle. Our study attempts to bring these issues in land modeling to the forefront, and are analogous with ongoing improvements in other components of earth system models (e.g., Wan et al., 2016)

Comment 29: Calibration is another issue. You need to calibrate ALM with each of five approaches properly. If we take any model, and replace part of this model with the formulation from another model, there will be almost infinite number of studies of this kind. The question is how useful this kind of study really is?
Response: As we explained previously, calibration is irrelevant in this study, given the similar model behavior in the historical period when comparing our models and the default CLM4.5/ALMv0. And we stress again that it is not a good approach to calibrate an inappropriately implemented model to make it better match observations. We have added text to the revised manuscript to clarify this issue (P3: L11-12).

Comment 30: The fonts used in the manuscript are hardly readable, quality of several figures are poor (1, 4, 5).
Response: We followed the EGU Copernicous template in preparing our manuscript, and the font size was set as small. We revised Figures 4 and 5 for color consistency. Otherwise, we think Figure 1 is sufficiently clear to serve its purpose, and the other reviewer can read it clearly.

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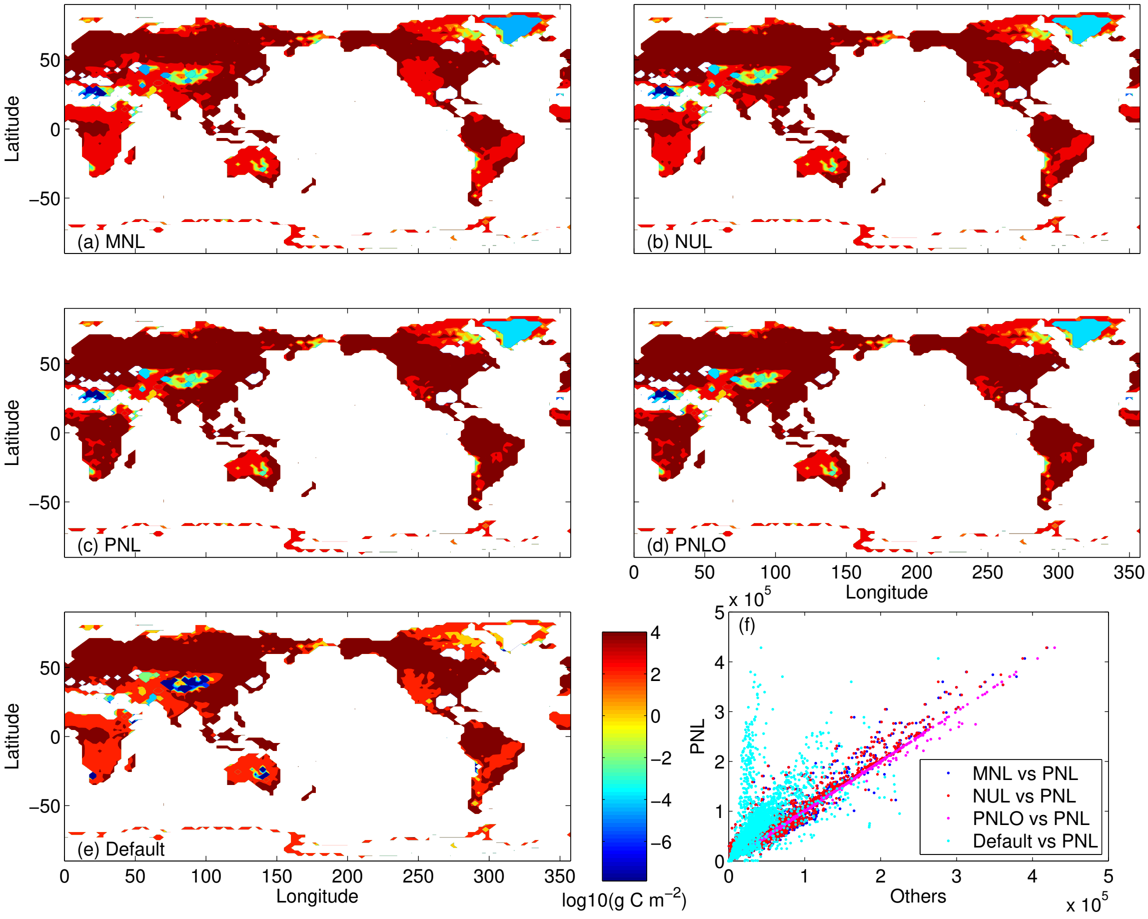

Figure X1. Comparison of initial soil carbon distributions that were for simulating the historical period.

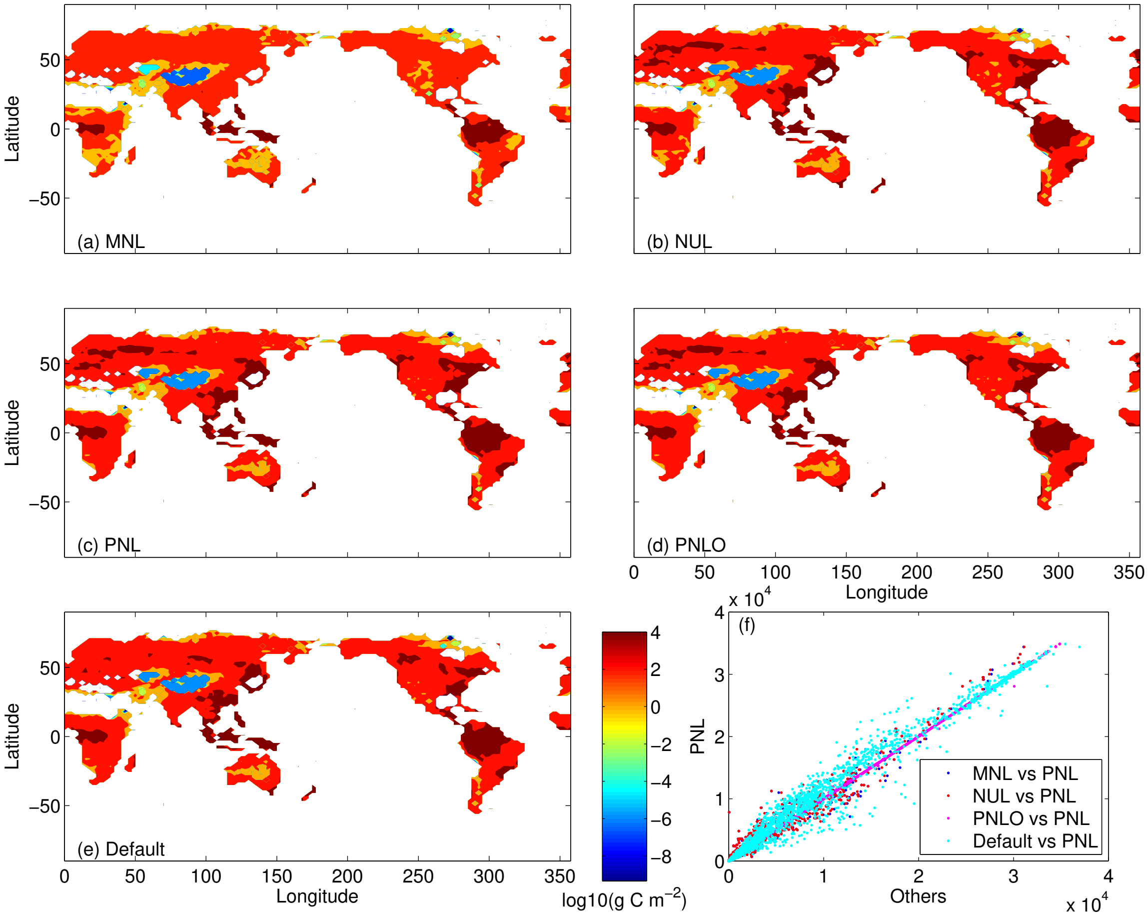

Figure X2. Comparison of initial vegetation carbon distributions that were for simulating the historical period.

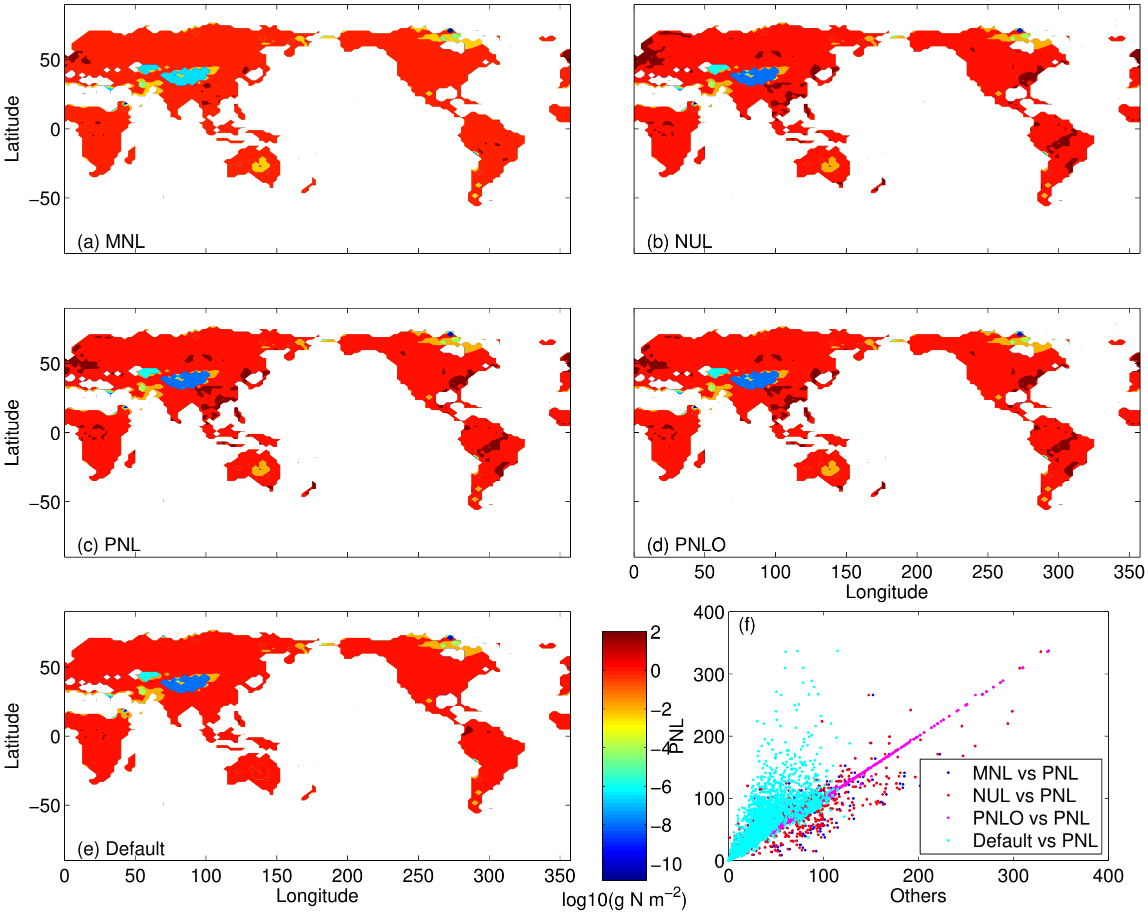

Figure X3. Comparison of initial vegetation nitrogen distributions that were for simulating the historical period.

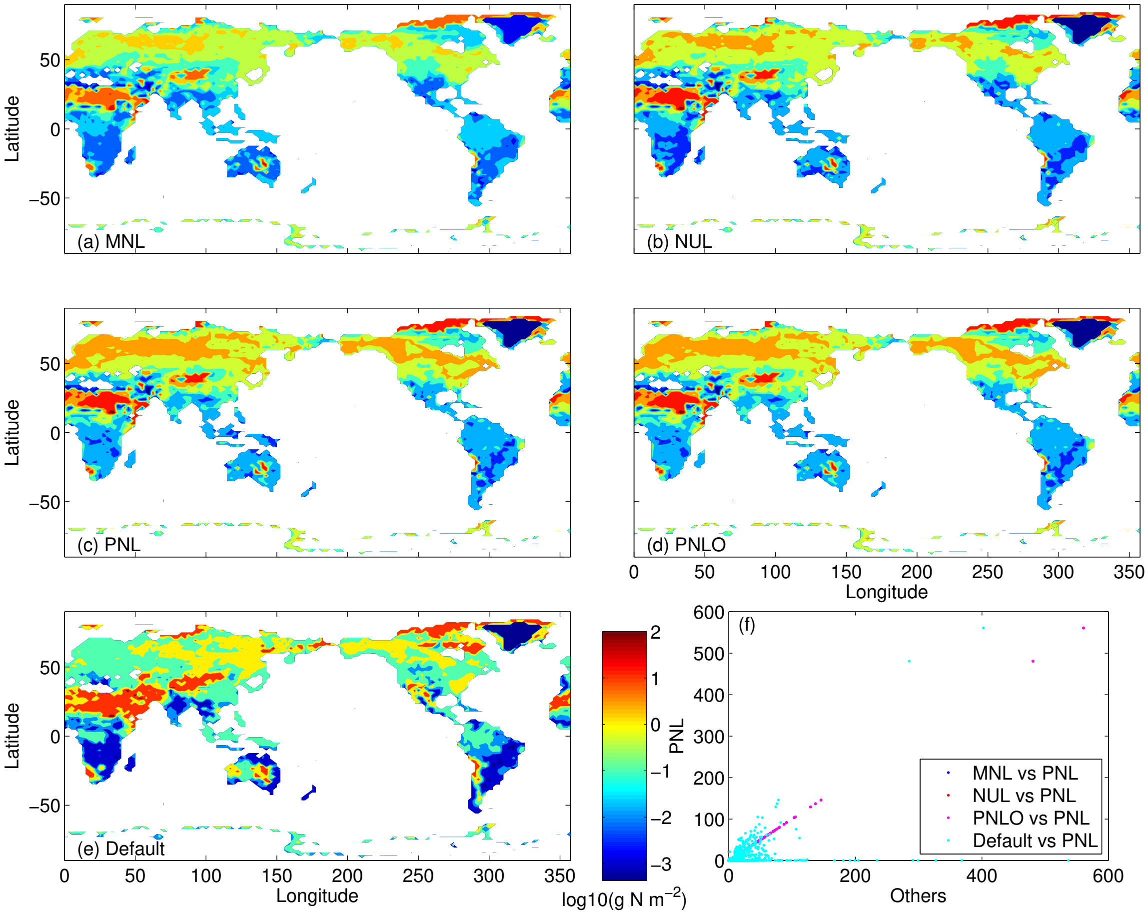

Figure X4. Comparison of initial soil mineral nitrogen distributions that were for simulating the historical period.

Potentially large uncertainty in ecosystem carbon dynamics resulting from ambiguous numerical coupling of carbon and nitrogen biogeochemistry: A demonstration with the ACME land model

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Abstract. Most Earth System Models (ESMs) have incorporated, or are incorporating, coupled carbon and nutrient dynamics in their land modules. We show here that different numerical implementations of nutrient controls may imply different ecological mechanisms not recognized in the original model design and can have first order impacts on predicted terrestrial carbon cycling. Using the version-zero land module of the DOE ESM ACME (ALMv0), we analysed land-atmosphere CO_2 exchange with coupled carbon and nitrogen dynamics through three commonly-applied numerical implementations of the supply-demand ansatz based nitrogen limitation: (1) Mineral Nitrogen based Limitation (MNL), (2) Net nitrogen Uptake based Limitation (NUL), and (3) Proportional Nitrogen flux based Limitation (PNL). By the last decade of the contemporary period (1850-2000), the three schemes resulted in very similar global terrestrial carbon and nitrogen distributions. However, under the RCP4.5 CO_2 concentration forcing, these implementations resulted in wildly diverging 2001-2300 land-atmosphere CO_2 exchanges. Quantitatively, the divergence is as large as that of the CMIP5 models by 2100 and is about 1900 Pg C (~890 ppmv) by 2300. Our analysis suggests that these differences result from: (1) the typically predicted high terrestrial ecosystem carbon to nitrogen ratios (i.e., nutrient constrained conditions), (2) the schemes predict different levels of limitations to the nitrogen-regulated processes, so that the PNL scheme favours larger nitrogen loss through aerobic and anaerobic denitrification and surface and subsurface hydrological transport and (3) the highly sensitive response of coarse woody debris dynamics to nitrogen limitation. We also found significant sensitivity of model predictions to initial conditions and numerical time step size but insignificant sensitivity to the sequence of numerical oxygen and nitrogen limitation or the ordering of calculation for reaction and chemical transport. We conclude that inconsistencies in numerical impositions of nutrient limitations have the potential to produce large uncertainties in predicted carbon stocks and long-term carbon-climate feedbacks. Finally, we recommend approaches to systematically alleviate these uncertainties.

Keywords: carbon-nitrogen feedbacks, nitrogen limitation, land-atmosphere CO_2 exchange, RCP4.5, law of the minimum

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1 Introduction

Earth System Models (ESMs) used for assessing future climate and related processes rely on large-scale land biogeochemical (BGC) models to simulate ecosystem responses to changing atmospheric CO$_2$, temperature, precipitation, nitrogen (N) deposition, and etc. Recent work analysing ESM land models that participated in the Coupled Model Intercomparison Project Phase 5 (CMIP5) showed very large differences among those models' predictions (e.g., Arora et al., 2013; Friedlingstein et al., 2014; Shao et al., 2013; Koven et al. 2015a). Such differences are often attributed to the four types of uncertainties, including structural (Tang et al., 2010; Wieder et al., 2015a), numerical (Yeh and Tripathi, 1989), parameterization (Tang and Zhuang, 2008; Luo et al., 2015), and forcing data (Clein et al., 2007; Blanke et al., 2016), which are, respectively, loosely related to the four stages of BGC model design: (I) conceptualizing the relevant mechanisms and translating them into governing equations; (II) numerical encoding of the governing equations; (III) process module calibration and parameterization; and (IV) model analyses and applications. There have been numerous examples of how one could quantify and reduce these uncertainties (e.g., Tang and Zhuang, 2008, 2009; Williams et al., 2009; Lichstein et al., 2014; Wei et al., 2014; Shi et al., 2015). Here we describe a new type of uncertainty that is a combination of type-I and type-II, and can result in predictions of ecosystem carbon dynamics as divergent as that of CMIP5 land models.

We report our findings using the carbon-nitrogen coupling as an example; however, this new type of uncertainty is related to the broader issue of carbon-nutrient coupling in all kinds of BGC models. Specifically, it relates to how one should numerically represent the fact that different substrates can limit ecosystem biogeochemical processes under different conditions. For instance, it is believed that many terrestrial ecosystems are nitrogen limited (Vitousek and Howarth, 1991; LeBauer and Treseder, 2008), because breaking down the triple bond of dinitrogen (N$_2$) and converting it into assimilable forms requires a significant fraction of newly assimilated or reserved carbon (Gutschick, 1987). Tropical forest ecosystems are often regarded as phosphorus limited because of their highly weathered soils (Walker and Syers, 1976), but nitrogen or even carbon or potassium limitation can still occur (e.g., Wright et al., 2011; Fanin et al., 2015). In moist environments, such as wetlands, where organic matter decomposition is more likely oxygen limited, anaerobic decomposition dominates but aerobic decomposition may proceed simultaneously (DeBusk et al., 2001). Given this wide range of substrate limitation conditions, it is therefore logical to ask: how would different numerical treatments of substrate limitation influence the prediction of a land BGC model?

We answer the above question by focusing on nitrogen—the most important macronutrient related to whether or not terrestrial ecosystems could continue to sequester anthropogenic CO$_2$ (Oren et al., 2001; Drake et al., 2011; Grant, 2013). Following Kovarova-Kova and Egqli (1998)'s use of terms "growth-controlling" and "growth-limiting" in substrate dynamics, we note there are two aspects that determine the modelled influence of nitrogen on ecosystem carbon dynamics: (1) the mechanistic formulation of carbon and nitrogen coupling (i.e. growth-controlling) and (2) the numerical implementation of a given formulation (i.e. growth-limiting). The first aspect regards the analytical formulation of how one or more nutrients mechanistically limit the growth of an organism or a compartment of an organism. We acknowledge that

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there has been no consensus on how this should be done, and many opinions are currently under debate (e.g., Kooijman, 1998; Parida, 2011; Agren et al., 2012; Niu et al., 2016; Stocker et al., 2016; Zhu et al., 2016). Therefore, we will present our opinion on this first aspect elsewhere, although some of that has been alluded in Tang and Riley (2013), Zhu and Riley (2015) and Zhu et al. (2016). The second aspect concerns how the coupling between different components as given in an analytical formulation should be achieved in a numerically consistent manner. This second aspect has been rarely discussed in the field of land biogeochemical modelling; event though similar issues (called as multi-physics coupling) have been scrutinized in other branches of earth system modelling. A few excellent examples are Phillips (1956), Arakawa (1965) and Wan et al. (2016) for atmospheric physics, Sandu (2001), Nguyen et al. (2009) and Wan et al. (2013) for atmospheric chemistry, Tang et al. (2015) for soil-plant hydrology and Broekhuizen et al. (2008) for marine biogeochemistry. In a nutshell, all these studies indicate that an inappropriate numerical implementation could render an analytically well-formulated model to behave unrealistically, and calibrating and applying such models (in terms of doing steps III and IV as identified above) will be a waste of resources (as implied in the Lax equivalence theorem (Lax and Richtmyer, 1956)).

For this study, we begin our analysis with the following equation for a generic substrate S in a soil control volume:

$$\frac{dS}{dt} = F_{S,input} - F_{S,uptake} \tag{1}$$

where $F_{S,input}$ and $F_{S,uptake}$ are, respectively, substrate input (from all sources) and substrate uptake (by all competing entities). Here and below, unless otherwise stated explicitly, we assume the units of all variables in a given equation are consistently defined. To simplify the discussion, we have solved the overall spatiotemporal evolution of substrate S (which is a function of both transport and biogeochemistry) using the operator splitting approach (e.g., Strang, 1968; Tang et al., 2013), so that $F_{S,input}$ and $F_{S,uptake}$ in equation (1) only refer, respectively, to substrate release and uptake from the interacting agents. As such, for the substrate S (i.e. mineral nitrogen) that we are interested in (note we henceforth use S and mineral nitrogen interchangeably unless a clarification is required), input $F_{S,input}$ is microbial nitrogen mineralization from soil organic matter (SOM) decomposition; while $F_{S,uptake}$ includes plant nitrogen assimilation (to support growth) and microbial nitrogen utilization (to support decomposition, nitrification and denitrification). If the interaction between soil mineral surfaces and ammonium nitrogen is considered (e.g. Gerber et al., 2010), $F_{S,input}$ and $F_{S,uptake}$ should be modified accordingly, depending on whether ammonium is adsorbed or desorbed from soil minerals. With the operator splitting approach, nitrogen input from other sources (including fertilization, atmospheric nitrogen deposition, nitrogen fixation) and losses through hydrological transport are integrated separately from the competitive coupling between nitrogen mineralization and assimilation. We have tested this treatment by switching the order between solving the biogeochemical processes and transport and found the ordering affected the results marginally small.

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When solved with the forward Euler scheme (e.g. Atkinson, 1989), Equation (1) may be approximated as:

$$S(t+\Delta t)=S(t)+\left(F_{S,input}-F_{S,uptake}\right)\Delta t \tag{2}$$

With a given numerical time step Δt, if $S(t+\Delta t)$ becomes negative (before any adjustment to the rates that change $S(t)$), the biogeochemical system is defined as substrate-S limited during that numerical time step. Here we once again remind readers not to confuse this definition (of growth limiting substrate) with using different analytical formulations of how nutrients could limit or co-limit the biogeochemical system (i.e. growth-controlling substrates), because this numerical limitation (i.e. growth limiting substrate) will always occur for whatever analytical formulation (of growth controlling substrates) being used. We also note that this numerical definition of nitrogen limitation (which operates on time scales from minutes to hours) appears different from the ecological definition, which is defined as stimulated ecosystem productivity in response to nitrogen addition and operates on time scales from days to years (Vitousek and Howarth, 1991). However, in a BGC model, ecological nitrogen limitation is realized as an emergent response accumulated from many within time-step nitrogen limitations (and should be considered as a combination of growth-controlling and growth-limiting processes).

Using a higher order numerical scheme will not avoid this numerical substrate limitation, and, when substrate limitation occurs, the high order scheme will usually become first order (Bolley and Crouzeix, 1978), a result that also holds for implicit schemes (Hundsdorfer and Verwer, 2003). Higher order accuracy may be achieved if both the substrate production and destruction rates are modified simultaneously (e.g., Burchard et al., 2003), but such an approach will fail when substrate production is independent of consumption, a situation that occurs exactly in the CENTURY-like soil biogeochemical models (Parton et al. 1988; Koven et al. 2013), where, because the different soil organic matter pools are decayed in a linearly dependent manner, the activity of nitrogen mineralizers is independent from that of nitrogen immobilizers (Tang and Riley, 2016). Nor will an adaptive time stepping approach resolve this numerical substrate limitation problem, because in many cases it would require an impractically small time-step to avoid negative numerical solutions (Formaggia and Scott, 2011). Nevertheless, a numerical nitrogen limitation as applied in equation (2) does depend on the time step size, but as we demonstrate below, this uncertainty is secondary to that from using different numerical implementations of the supply-demand ansatz based nitrogen limitation.

We now analyse three legitimate and commonly applied numerical methods to resolve substrate limitation when solving equation (2). We reveal that the three numerical approaches imply different coupling between nitrogen competitors and producers in the model, they therefore lead to different (sometimes unacknowledged) ecological coupling between carbon and nitrogen dynamics.

The first nitrogen uptake limitation approach has been adopted by models like CLM-CNP (Yang et al., 2014), BiomeBGC (Thornton et al., 2002), BiomeBGC MuSo (Hidy and Barcza, 2014), JSBACH-CN (Parida, 2011; with

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denitrification excluded from $F_{S,uptake}$), CLM4.0 (Oleson et al., 2010), CLM4.5 (Oleson et al., 2013), and one version of ALMv1 (the land model in the DOE earth system model ACME-v1). Mathematically, it reads

$$\overline{F}_{S,uptake} = \min\left\{ \frac{S(t)/\Delta t}{F_{S,uptake}}, 1 \right\} F_{S,uptake} \tag{3}$$

Equation (3) assumes that the actual total nitrogen uptake $\overline{F}_{S,uptake}$ is limited solely by the available mineral nitrogen $S(t)$ and is not affected by mineral nitrogen released from SOM decomposition during the numerical time step, which is certainly inconsistent with the governing equation. In the following, we name this approach (i.e., equation (3)) as the **M**ineral **N**itrogen based **L**imitation scheme (MNL).

In some models, like CABLE (Wang et al., 2010) or the Generic Decomposition and Yield model (Comins and McMurtrie, 1993), the *j*-th sub-component $F_{S,uptake,j}$ of $F_{S,uptake}$ may already include substrate limitation based on the availability of $S(t)$. These models apply either equation (3) or its variants (to be introduced later), or a "numerical" Monod term (e.g., Tang et al., 2016) that has no chemical or biological kinetic meaning (as in contrast to the enzymatic Monod function) to the *j*-th potential uptake flux $F_{0,S,uptake,j}$. When both nitrogen and phosphorus are considered for an entity of fixed stoichiometry (e.g., a decomposing organic matter pool or a microbe), the imposition of substrate limitation is even more uncertain. One approach is to use the potential nitrogen uptake flux $F_{0,N,uptake}$ and phosphorus uptake flux $F_{0,P,uptake}$ to first calculate the nitrogen-limiting factor x_N and phosphorus-limiting factor x_P

$$x_N = \min\left\{ \frac{MIN_N/\Delta t}{F_{0,N,uptake}}, 1 \right\} \tag{4}$$

$$x_P = \min\left\{ \frac{MIN_P/\Delta t}{F_{0,P,uptake}}, 1 \right\} \tag{5}$$

Then Liebig's law of the minimum is applied by taking the minimum of x_N and x_P to compute an overall limiting factor x_{NP} that constrains the overall decomposition flux, which by stoichiometry balance will lead to down-regulated nitrogen and phosphorus uptake rates $F_{N,uptake,j}$ and $F_{P,uptake,j}$ that are then used to resolve the nitrogen and phosphorus competition. Occasionally, x_N and x_P may be calculated using Monod functions for each of the substrate competing entities, leading to

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a premature application of the law of the minimum onto the individuals (e.g., Leon and Tumpson, 1975; Danger et al., 2008). However (as we explained in Appendix A), such an application of the 'law of the minimum' mistakes the system-wise nutrient limitation as a local constraint on subcomponents (or individuals) of the system. Given the limited amount of nitrogen and phosphorus available for competition, an additional application of either equation (3) (or the to be introduced equations (6) or (7)) may still be imposed to avoid negative numerical solutions when all competing fluxes are resolved (i.e., a second application of the law of the minimum will be introduced automatically through the numerical integration). Such a strategy then leads to a double counting of nutrient limitation if the mass balance is imposed strictly (we note such double counting is different from that discussed in Downing et al. (1999) for phytoplankton fertilization experiment), and if the mass balance is not imposed strictly, an unwanted numerical nutrient fertilization might occur (e.g., the ODE45 solver as demonstrated in Tang and Riley (2016)).

The second nitrogen limitation scheme that we analyse here is represented as:

$$\overline{F}_{S,uptake}=\min\left\{\frac{S(t)/\Delta t}{F_{S,uptake}-F_{S,input}},1\right\}F_{S,uptake} \tag{6}$$

We name equation (6) the **N**et nitrogen **U**ptake based **L**imitation (NUL) scheme (note when NUL is applied, it holds that $F_{S,uptake}-F_{S,input}>0$). The NUL scheme is based on the approach of derivative clipping, and is used in MATLAB's ODE45 (Shampine et al., 2005). However, ODE45 imposes equation (6) by violating the law of mass balance (Tang and Riley, 2016). We avoid this problem here by applying the flux adjustment only to $F_{S,uptake}$, because $F_{S,input}$ (as it asspears in ALMv0) is assumed independent from substrate S in equation (6).

The third nitrogen limitation scheme is

$$\overline{F}_{S,uptake}=\min\left\{\frac{F_{S,input}+S(t)/\Delta t}{F_{S,uptake}},1\right\}F_{S,uptake} \tag{7}$$

We name equation (7) as the **P**roportional **N**itrogen flux based **L**imitation (PNL), and it is the only numerical scheme (among the three we analysed) that is consistent with the governing equation (which can be verified by entering equation (7) into equation (2) and observing as required that $S(t+\Delta t)=0$ when $S(t)$ is limiting). PNL assumes that the newly (i.e., within the time step) released mineral nitrogen ($F_{S,input}$) and existing (i.e., at the beginning of the time step) mineral nitrogen $S(t)$ are equally accessible to immobilizers. This assumption is an oversimplification because diffusion can limit the newly released and existing mineral nitrogen from mixing completely in the soil over the typically short time steps in land models (0.5 – 1 h) (Schimel and Bennett, 2004). Therefore PNL will underestimate the true nitrogen limitation. We also note that

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when diffusion limitation is ignored, assuming whether or not plants and microbes have absolute priority of newly released mineral nitrogen over existing mineral nitrogen will not change the form of equation (7). A modified PNL scheme that includes diffusion constraints is used in the *ecosys* model (e.g. Grant, 2013) to rectify overly large nutrient uptake fluxes (personal discussion with R. Grant, 2016) that can lead to negative nutrient concentrations.

There have been other numerical schemes proposed for nitrogen limitation (which however will not be analysed in this study). For instance, Wang et al. (2010) in their constraint of decomposition due to nitrogen limitation (cf. their equation C12) calculated the de facto decomposer nitrogen uptake as

$$\bar{F} = \min\left\{\max\left\{1+\frac{\left(F_{S,input}-F_{S,uptake}\right)\Delta t}{S\left(t\right)},0\right\},1\right\}F_{S,uptake} \tag{8}$$

where $F_{S,input}$ and $F_{S,uptake}$ refer, respectively, to nitrogen mineralization and microbial nitrogen immobilization. Equation (8) reduces nitrogen uptake when the net mineralization $F_{S,input}-F_{S,uptake}$ is negative, and has no effect on nitrogen uptake when net mineralization is positive (we acknowledge that equation (8) is a more complete form with respect to their equation C12 because their equation C12 was only applied to negative net nitrogen mineralization). But as we explained above, this approach will not avoid predicted negative nitrogen concentrations and further adjustments as represented in the MNL, NUL or PNL scheme are needed.

Numerically, MNL, NUL, and PNL are all (seemingly) legitimate approximations to the same governing equation (1) as discretized in the forward Euler form equation (2) (type-II uncertainty). They nevertheless represent different biogeochemical coupling between mineral nitrogen, plants, and microbes (type-I uncertainty). When the actual numerical representation of nitrogen limitation is not explicitly reported (which is common in the literature), one would regard the BGC models using these three schemes as structurally identical and numerically similar (and indeed for nitrogen unlimited conditions, these three approaches lead to identical model predictions (Tang and Riley, 2016)). However, because ecosystem carbon sequestration is the difference between several large magnitude nitrogen-limited ecosystem carbon fluxes, we hypothesize that different numerical nitrogen limitation schemes will lead to different predictions of ecosystem carbon dynamics.

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We therefore in this study address two hypotheses:

(H1): The ambiguous numerical implementation of nitrogen limitation will lead to large uncertainty in simulated ecosystem carbon dynamics.

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(H2): Uncertainty from the model time-step size is smaller than that resulting from the use of different nutrient limitation schemes.

We evaluated the above hypotheses using the ALMv0 model that integrates BeTR—a numerically robust reactive transport module (RTM) for biogeochemical transport and reactions (Tang et al., 2013)—with simulations of both historical

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and future RCP4.5 emission scenario atmospheric CO_2 forcing. We compared our simulated uncertainty to that reported for the CMIP5 models (Shao et al., 2013), and assert H1 as true when these two sets of experiments are of comparable spread in terms of NEE (net ecosystem exchange of carbon). H2 is asserted as true if the site-level simulations indicate the time-step size affects the simulation less than using different numerical implementations as indicated in equations (3), (6) and (7). Below we describe the model configurations and simulation protocols, present and discuss our model results, and finally give recommendations on how to remove or alleviate this new type of uncertainty (i.e., ambiguous numerical nutrient limitation).

2. Methods

2.1 Model configuration

We applied ALMv0-BeTR to explore how different numerical schemes of nitrogen limitation affect the predicted ecosystem uptake of atmospheric CO_2. BeTR is a multiphase RTM that consistently represents the transport (including multiphase diffusion, advection, ebullition, and gas phase arenchyma transport) for an arbitrary number of chemical tracers, which for this study includes seven carbon pools (Koven et al., 2013), and eight abiotic tracers, N_2, O_2, Ar, CH_4, CO_2, NH_4^+, N_2O, and NO_3^-. Compared to the first version of BeTR in CLM4 (Tang et al., 2013), ALMv0-BeTR improves the numerical treatment of dual phase diffusion (Tang and Riley, 2014) and advection (Manson and Wallis, 2000) (see Figure S1 for a demonstration of its numerical accuracy in tracer transport), and uses F90's object oriented polymorphism to implement different BGC formulations within the same biophysical environment. As in the default ALMv0 BGC, which is the de facto CLM4.5BGC (Koven et al., 2013; Oleson et al., 2013), all BeTR BGC implementations do not physically transport NH_4^+. We implemented the biogeochemistry of all BeTR BGC models using the Peterson matrix based formulation (Russell, 2006; Tang and Riley, 2016), so that minimal modification was needed to implement the three nitrogen limitation schemes (i.e., MNL, NUL, and PNL).

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We note that ALMv0/CLM4.5BGC uses an instantaneous, supply-demand ansatz (SDA; Parida, 2011) for downregulating GPP. Under nitrogen-limited conditions, this approach first calculates the ratio between existing soil mineral nitrogen pool and total potential nitrogen uptake (by plants and microbes) to avoid negative mineral nitrogen stock, and then multiplies this ratio with the nitrogen unlimited GPP to obtain the down-regulated GPP (Parida applied this approach to NPP though). This anasatz approach unrealistically assumes that root nutrient uptake instantaneously affects leaf photosynthesis and artificially restricts the plant and microbial nutrient competition to occur before plant carbon allocation. We recently showed that this approach (1) leads to very unrealistic diurnal GPP cycles (Ghimire et al. 2016) and (2) has not been corroborated by observations (Zhu et al., 2016), even though it may be ecologically convenient for analysing long-term ecosystem biogeochemistry with a time step of years. We therefore removed this down-regulation scheme in all BeTR BGC

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simulations by adding a nitrogen storage pool to fulfil the nitrogen demand from GPP and refill the nitrogen storage pool through plant uptake (in presence of microbial competition).

ALMv0/CLM4.5BGC employs a fixed CN stoichiometry for plants and a CENTURY-like (Parton et al., 1988) formulation for soil BGC, where the latter represents microbial population dynamics and associated biogeochemical activity implicitly. All models used here allow plants and microbes to compete equally (or proportionally) for NH_4^+ and NO_3^-, and assume that both plants and organic matter decomposers assimilate NH_4^+ over NO_3^-. The first assumption (on whether the uptake of NH_4^+ and NO_3^- is proportional to their pool sizes) is now under intense debate (e.g., Gerber et al., 2010; Zaehle and Friend, 2010; Thomas et al., 2015; Niu et al., 2016; Zhu et al., 2016), whereas the second assumption is very likely unrealistic because (1) it restricts the model to execute nitrogen limitation after oxygen limitation (as NO_3^- demand by denitrifiers is a function of oxygen and applying nitrogen limitation requires knowing the relative uptake demand of NH_4^+ over NO_3^-), even though they occur simultaneously in the real world and (2) a grid cell in any large scale BGC model actually represents the average of a heterogeneous soil, so the uptake of NO_3^- should never be zero as long as some NO_3^- exists.

To evaluate hypothesis (H1), we used five BGC model configurations implemented in ALMv0-BeTR (Table 1). Among them, the three BGC formulations (MNL, NUL, and PNL) differ in their numerical interpretations of nitrogen limitation. Since all model configurations in BeTR require identical model inputs, we also tested the model sensitivity to initial conditions by comparing PNL with PNLIC, where the latter uses the code base of PNL and initial conditions from the NUL simulation. Simulations PNLIC and NUL are compared to demonstrate the effect of different nitrogen limitation implementations with the same initial conditions. The final model configuration, PNLO, when compared to PNL, illustrates the ordering dependence of substrate limitation (for oxygen and nitrogen). To prevent the model PNLO from crashing (on negative values of oxygen or mineral nitrogen), we first predicted the relative demand for NH_4^+ and NO_3^- based on total mineral nitrogen availability, then implemented oxygen limitation on nitrification and decomposition, and finally applied nitrogen limitation to microbes and plants a second time to obtain the corrected nitrogen uptake for plants and microbes. This requirement to apply nitrogen limitation in a predictor-corrector manner is not easily observable from the governing equations of the BGC model and demonstrates (1) that the default ALMv0/CLM4.5BGC model structures of plant-soil nitrogen interactions are problematic and (2) (once more) that numerical implementations of nutrient limitations in ESM land models may imply (sometimes unacknowledged) different ecological dynamics that is not described in the governing equations. We run our global simulations from 1850 to 2300 (see simulation protocol) and compare the output from 2006-2100 to the reported NEE for CMIP5 simulations (Shao et al., 2013) to evaluate H1.

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The second hypothesis (H2) is evaluated with four example single gridcell simulations in geographically and climatically distinct locations (Figure 3): (74.67°W, 40.6°N; Eastern U.S.), (26.22°E, 67.7°N; Northern Finland), (50.02°W, 4.88°S; North East Brazil), and (51.5°W, 30.0°S; South Brazil). These gridcells were chosen to illustrate spatial heterogeneity in how time stepping strategies would influence simulated ecosystem carbon dynamics. We adopted the strategy from Tang and Riley (2016) (their appendix D) for adaptive time stepping and designated relevant simulations with PNL-adapt. H2 is evaluated by comparing the effect of adaptive-time stepping to that of using different numerical implementations of nitrogen limitation.

2.2 Simulation protocol

All model simulations were first run to preindustrial equilibrium using the spinup protocol in Koven et al. (2013) with the QIAN climate forcing data (cycled for 1948-1972; Qian et al., 2006). The model output by the end of spinup was then used for simulations in the contemporary period 1850-2000 with diagnostic atmospheric CO_2 concentrations. The RCP4.5 scenario atmospheric CO_2 concentrations (starting from 2006; see Figure S2b) were used together with the cycled QIAN climate forcing for the simulation period 2001-2300. We did not apply the climate anomaly representing future climate change to the RCP simulations; therefore the simulated carbon dynamics over 2001-2300 only represented the effects of changing atmospheric nitrogen deposition (Figure S2a), atmospheric CO_2 (Figure S2b), and land use change. We expect that including more uncertainty sources (such as uncertain future climate) will further strengthen the conclusions of our study (e.g. Tang and Zhuang, 2008). We finally note that the decision to run the simulations to 2300 is inspired by Randerson et al. (2015) and is just to push the models to one type of extreme and see if they would behave unexpectedly.

3 Results

3.1 Global simulations for the contemporary period 1850-2000

For the last decade (1991-2000) of the historical simulation period 1850-2000, the six model simulations gave very similar latitudinal distributions of several important variables (Figure 1). Small differences were found for latitudinal distributions of total soil organic carbon (Figure 1f), total soil organic nitrogen (Figure 1g), total vegetation carbon (Figure 1h) and total vegetation nitrogen (Figure 1i). Particularly for the July latent heat flux (Figure 1e), all simulations overlap, which is consistent with the relatively small differences in July leaf area index (LAI), GPP, NPP, and total vegetation carbon (Figure 1b, c, d and h) and that plant transpiration has a fast response to climate forcing (which is the same in all six model simulations). The overall close agreement between the default simulation (purple line) and all five BeTR-based simulations indicates that (1) the BeTR-based simulations are behaving in a reasonable way as compared to ALMv0 and (2) it requires a long time for the effect of different nitrogen limitation schemes to emerge in the simulations. This second observation is consistent with the usually high ecosystem carbon to nitrogen ratio and that ecosystem carbon stocks are cumulative

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differences between the large fluxes of ecosystem carbon uptake (i.e., GPP) and ecosystem carbon loss (respiration and disturbances).

In contrast to the high degree of similarity between many of the variables simulated by the five BeTR-based models, the historical trajectories of cumulative NEE (positive means emitting CO_2 into the atmosphere) are very different (Figure 1a). Among the MNL, NUL, and PNL simulations, PNL (red line) had higher land carbon release compared to NUL (green line; an almost carbon neutral land by year 2000) and MNL (blue line; a cumulative land carbon uptake of about 40 Pg C by year 2000). The cumulative NEE simulated by PNLO (black line) is very similar to that by PNL, yet the ordering dependence still lowered the cumulative carbon release by about 50 Pg C compared to PNL by year 2000. PNLIC (cyan line) showed an anomalously high release of land carbon resulting from enhanced decomposition of coarse woody debris (Figures S3-a1, b1, and c1), which is reflected in the higher heterotrophic respiration (Figure S4c) driven by more efficient decomposer nitrogen immobilization in PNL as compared to NUL. Although an in depth analysis will be provided using point simulations (section 3.3), this more efficient nitrogen uptake by PNL can be simply explained by observing the similar nitrogen input from fixation and deposition between the models (results are not shown but can be inferred from the almost overlapping NPP, which controls nitrogen fixation in this version of ALM), and (as shown mathematically in Supplemental Material) that the nitrogen uptake calculated from equation (6) (for NUL) is smaller than that from equation (7) (for PNL). The huge difference between PNL and PNLIC in the cumulative NEE (Figure 1a) indicates that the CENTURY-like BGC model is very sensitive to initial conditions, corroborating the finding in Exbrayat et al. (2014). Finally, we observed very small differences in the latitudinal distributions of soil mineral nitrogen over 1991-2000 between the five BeTR-based simulations, and those concentrations are lower than that simulated by the default model (Figure S5).

3.2 Global simulations for the period 2001-2300

Although having very similar carbon and nitrogen stocks for the decade of 1991-2000 (Figure 1), the five BeTR simulations driven by the RCP4.5 atmospheric CO_2 concentrations diverged into three groups for 2001-2300 (Figure 2). For the north temperate region (i.e., north of 23.2° N and south of 66.3° N; Figure 2a1), simulations NUL and MNL almost overlapped and predicted a carbon gain of about 250 Pg C (~3200 g C m^{-2}) by year 2300; simulations PNLO and PNL almost overlapped and predicted a carbon gain of about 110 Pg C (~1400 g C m^{-2}) by year 2300; and PNLIC predicted a small carbon loss of about −380 Pg C (~ −4900 g C m^{-2}) by year 2300. The tropics (defined as the region between 23.2° S and 23.2° N) showed larger divergence (Figure 2b1) with a high carbon gain predicted by MNL about 1180 Pg C (~19000 g C m^{-2}) and NUL about 1150 Pg C (~18700 g C m^{-2}) by year 2300, and a lower carbon gain by PNL about 360 Pg C (~5800 g C m^{-2}) and PNLO about 320 Pg C (~5200 g C m^{-2}), and about −6 Pg C (~−100 g C m^{-2}) loss by PNLIC. The divergence in the Arctic region (defined with latitudes north of 66.3° N; Figure 2c1) is smallest among the three regions, with a high carbon gain about 16 Pg C (~ 1400 g C m^{-2} by MNL and NUL), a small carbon gain about 4 Pg C (~ 340 g C m^{-2} by PNL and PNLO), and a large carbon loss about −14 Pg C (~ −1200 g C m^{-2}) by year 2300.

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While we do not place high confidence on the predicted numerical value (as discussed previously and below), the global terrestrial carbon stocks change (Figure S6) between 2006 and 2100 spreads from 10 Pg C (weak sink; PNLIC) to 680 Pg C (sink; MNL), which approximately encapsulates the range (22~456 Pg C) reported in Shao et al. (2013) (their Table 4) for the CMIP5 simulations. By 2300, the predicted global terrestrial carbon stock change ranges from a source of about −390 Pg C (PNLIC) to a carbon sink of about 1500 Pg C (with MNL being slightly higher than NUL). We note that this 1500 Pg C sink is close to a reduction of 700 ppmv atmospheric CO_2 which is greater than the 550 ppmv atmospheric CO_2 forcing. This clearly indicates that the BGC model structure of ALMv0 is questionable (and so we don't place a good confidence on these numbers). Terrestrial carbon stock changes for the PNL and PNLO simulations fall between the predictions by PNLIC and MNL, with a carbon sink of 520 and 480 Pg C, respectively (Figure S6a). Since nitrogen limitation quantitatively increases across the model configurations (PNL < NUL < MNL), the sequential increases in carbon uptake (MNL > NUL > PNL) in response to the RCP4.5 atmospheric CO_2 trajectory imply that ALMv0 and CLM4.5BGC (which both use the MNL scheme) may predict too strong global CO_2 and nitrogen fertilization effects. We acknowledge that this stronger CO_2 fertilization effect resulting from stronger nitrogen limitation (as implied in the numerical implementations; see Supplemental Material) may first appear counter-intuitive, yet it can be reasonably explained through relevant ecological mechanisms (which lead to a stronger increase in heterotrophic respiration than in NPP under more efficient nitrogen uptake; see discussion in section 4.1). We also found that the predicted total soil carbon change is more sensitive than the total vegetation carbon change (Figure 2 and Figure S6) in response to the different nitrogen limitation implementations, indicating stronger nitrogen regulation of soil carbon stocks.

3.3 Point simulations for the four sites

For the group of simulations conducted at the four grid points (Figure 3), we observed similar divergences as those in the global simulations (Figure 2): the MNL scheme (blue lines) predicted higher carbon gain than did the PNL scheme (red lines), yet the NUL predictions (green lines) almost overlapped with those by MNL. Invoking adaptive time-stepping (PNL-adapt; magenta lines) further decreased the predicted carbon gain, which could be explained by the even more effective nitrogen uptake implied by the PNL scheme under smaller time steps. We also switched the computing order between reaction and transport for PNL-adapt (which like all simulations reported in this text calculates biogeochemical reaction before transport) and only found negligible difference (Figure S9).

3.4 Results of hypotheses evaluation

Taking all simulations together, we conclude that hypothesis H1 is affirmed given the spread of our simulated cumulative land carbon uptake is larger than that in Shao et al. (2013) for CMIP5 models. Meanwhile, H2 is satisfied in some, but not other, sites and that the size of the numerical time step could have either significant (Figure 3a) or secondary (Figure 3b, c, and d) importance on simulated ecosystem carbon stocks trajectories.

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4. Discussion

Below we first discuss how the three different numerical implementations of nitrogen limitation led to different partitioning of nitrogen fluxes. Then we explore the importance of the coarse woody debris in affecting the simulated spread in land-atmosphere carbon exchange. Finally we give our recommendations on how to alleviate the type of uncertainty we identified in this study.

4.1 Reasons for the large C cycle differences between different nitrogen limitation implementations

We observed that PNL, NUL, and MNL schemes predict sequentially stronger nitrogen limitation under the same mineral nitrogen availability (Supplemental Material). For biogeochemical models like ALM that resolve mineral nitrogen into ammonium and nitrate (together with the assumed preference of ammonium over nitrate), this order of limitation translates into sequentially less effective plant and microbial assimilation of ammonium and stronger uptake of nitrate nitrogen. Indeed, we found PNL-adapt predicted the highest nitrification rate (as nitrifiers are competing for ammonium in ALM) followed by PNL and MNL (which overlapped with NUL; see Figure 4a1, b1, c1, a2, b2 and c2), leading to the same ranking of soil nitrate abundance (Figure S10) and nitrate loss through aqueous transport (Figure 4a4, b4, and c4). The difference in denitrification rates as simulated by different nitrogen limitation schemes is also evident, with the lowest value predicted by PNL-adapt, and increasing in MNL (which overlaps NUL) and then PNL. The simulations at 51.5° W, 30.0 ° S (which ALM identifies as a C_3 grassland) only qualitatively resemble those at the other three sites, yet the ranking of soil nitrate abundance remains (Figure S10d). Corresponding to the nitrogen dynamics, the ecosystem heterotrophic respiration also increases in the order of MNL (which overlaps NUL), PNL, and then PNL-adapt, except for the period after 1980 for the fourth site (Figure 5d), indicating a strong sensitivity of carbon dynamics to nitrogen processes. For global simulations driven by RCP4.5 atmospheric CO_2 forcing over 2001-2300, this stronger increase of respiration led PNL to predict about 3200 Pg C more respiration than did by MNL, yet the NPP predicted by PNL only increased by 1900 Pg C as compared to that by MNL, which together led the PNL scheme to predict a lower CO_2 fertilization effect.

4.2 High sensitivity of coarse woody debris dynamics to nitrogen

We observed that the response of coarse woody debris (CWD) pool dominated the simulated difference in total land-atmosphere carbon exchange during both the contemporary period 1850-2000 (Figure S3) and the projection period 2001-2300 (Figures S7 and S8). A smaller fraction is contributed from carbon in woody product and seed (see second rows of Figures S3, S7 and S8). In ALMv0/CLM4.5BGC, coarse woody debris is accumulated from mortality due to fire (predicted with the model by Li et al. (2012a, b)) and background death (2% per year; Oleson et al., 2013), harvest and land use change, and it is lost through decomposition into lignin and cellulose. The decomposition of CWD immobilizes nitrogen, and is assumed to produce no CO_2, where the latter is obviously contradictory to reality (e.g. Gough et al., 2007). Nevertheless, the more efficient nitrogen uptake as ranked in PNL, NUL and MNL (supplemental material) has led to the

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sequentially higher loss of CWD in the order of low to high as MNL, NUL, PNL (PNLO) and PNLIC (Figures S7 and S8). PNLIC has predicted the highest loss of CWD, because it uses the initial condition from NUL and NUL has accumulated more CWD during the spinup period due to its less efficient nitrogen uptake as compared to PNL. Regionally, the tropics showed the largest spread in the predicted CWD loss (−121~214 g C m^{-2} yr^{-1}), followed by the north temperate region (−156~10 g C m^{-2} yr^{-1}), south of 23° S (−10~8 g C m^{-2} yr^{-1}) and the Arctic (−4~2 g C m^{-2} yr^{-1}; see Figure S6 and S7). Such high sensitivity of the CWD dynamics with respect to the nitrogen dynamics further indicates urgency to develop robust implementations of nitrogen limitation in ESM land biogeochemical models.

4.3 Strategies for robust carbon and nitrogen coupling

Through the above results we show that ambiguous numerical implementation of nitrogen limitation could have led to a large carbon cycle prediction uncertainty. To rectify this situation, we have four recommendations (surrounding both the growth-controlling and growth-limiting processes) to help achieve a numerically robust coupling between carbon and nitrogen (or more generally nutrient) dynamics.

First and foremost, nutrient limitations should be handled automatically through a robust numerical solver (i.e. a better classification of the growth-limiting and growth-controlling processes), rather than being applied to individual processes through the convenient law of the minimum, an approach that has yet been challenged by observations (e.g. O'Neill, 1989; Danger et al., 2008), and is mechanistically redundant (appendix A). In reality, nutrient limitations emerge from continuous interactions among all entities and substrates in the ecosystem. Analytically applying law of the minimum to each of the modelled entities can turn the emergent limitation into a specific mechanism constraint that ignores interactions between competing entities. If a strategy is also employed to avoid (unphysical) negative numerical solutions (which is necessary), an unwanted double counting of substrate limitation will occur. Likewise, the numerical Monod-term based approach (e.g., Tang et al., 2016) incorrectly applies the nutrient limitation as an emergent constraint, as it introduces a specific mechanism constraint that depends on an ambiguously defined residual substrate concentration.

Second, we recommend models explicitly represent substrate kinetics for substrate competition between all consumers (i.e. better formulation of the growth-controlling process). On the one hand, substrate kinetics naturally have the property that as substrate concentrations decrease, uptake fluxes will smoothly decrease. On the other hand, unlike the numerical Monod term (in Tang et al., 2016; which can be equally replaced with functions like $S^n/\left(S^n+K_S\right)$, where n is the quantitative order and K_S is the numerical half saturation constant), appropriately applied substrate kinetics, e.g., the Equilibrium Chemistry Approximation (ECA) kinetics (Tang and Riley, 2013; Tang, 2015; Zhu et al., 2016), have a mechanistic underpinning for the interactions between entities involved in substrate dynamics. In particular, the ECA kinetics allows for an explicit formulation of entity interactions for each substrate, whereas the application of Michaelis-Menten kinetics will render representation of competitive pressures into the system-wise numerical constraint, possibly

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causing inconsistencies between the conceptual model, its governing equations, and the numerical solution (see the litter decomposition example in Tang and Riley (2013)).

Third, we contend that more robust numerical solvers should be employed to solve the BGC governing equations (i.e. better implementation of the growth-limiting process). Terrestrial biogeochemical modelling has traditionally not paid sufficient attention to this issue: model equations are often integrated with the single step Euler forward scheme (with a few exceptions such as the TEM model (Raich et al., 1992) and the ED model (Knox, 2012), which used multi-step methods such as the Runge-Kutta scheme), and ad hoc manipulations are invoked to rectify the unphysical numerical solutions (e.g., see discussions in Tang and Riley (2016)). This may not be a severe issue when the models are of low complexity (e.g., the CMIP5 models are mostly carbon-only models), where chances of unphysical solutions are less likely to occur. However, there are urgent scientific reasons to introduce more mechanisms into terrestrial biogeochemical models (e.g., Wieder et al., 2015b) for better and more comprehensive analyses of carbon-climate feedbacks. In particular, the migration from single-layer to vertically resolved models is required to correctly simulate global soil carbon stocks, especially for Arctic ecosystems (Koven et al., 2013, 2015b). For ecosystems such as peatlands, wetlands, rice paddies and tropical forests, the soil physical environmental will frequently fluctuate between wet and dry conditions, causing strong shifts in soil redox status. These dynamics will make the problem of substrate limitation more likely for different substrates over time. The first order explicit reaction-based flux back tracing algorithm proposed in Tang and Riley (2016) is helpful to avoid unphysical negative substrate concentrations during model execution and is numerically consistent with the processes represented in the governing equations (thus it satisfies the Lax equivalence theorem (Lax and Richtmyer, 1956)). However, its explicit time stepping approach may cause a ‘zigzag’ phenomena or premature convergence in some unusual cases (e.g., Figure S11). The implicit scheme may also have strong time stepping dependence, and for complex biogeochemical systems, clipping and variable transform may be needed for the implicit scheme to maintain positive solutions for concentrations (Tang et al., 2016). However, as we discussed, the clipping approaches can introduce mass balance errors into the model. One possible candidate to alleviate the time-stepping dependence is the exponential integrator (e.g. Tuckmantel, 2010), but it may still suffer from violating the strict mass balance constraint that is guaranteed in Tang and Riley’s approach. We will present our exercise of the exponential integrator elsewhere.

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Finally, we suggest that biogeochemical models should provide more transparent methods description for users to identify uncertainties (i.e. better documentation of the growth-controlling and growth-limiting processes), and then apply approaches to robustly test model structural uncertainty. In reviewing the literature, we rarely found sufficient information regarding how substrate limitation is numerically implemented in different models. Even when it is available, this information is usually buried within lengthy derivations of the governing equations, making it difficult to determine to what extent the numerical solutions are robust to the types of problems identified above. It is possible to organize a model’s governing equations into a set of clearly stated differential and algebraic equations, and solve them by simply invoking available numerical solvers. Such an approach will allow (1) a robust testing of how a model’s simulation depends on the numerical solver and (2) for assessment of model structural uncertainty if multiple models (or model realizations) are solved with the same robust numerical solver. Standardizing this component of land models could dramatically improve prediction uncertainty quantification and facilitate evaluation of new processes, leading to improved analysis of ecosystem dynamics and C-climate interactions.

5. Conclusions

The problems associated with ambiguous numerical implementation of substrate limitations are likely present in most ESM land models. Here, we used the coupled carbon-nitrogen dynamics in the version zero ACME land model as an example and demonstrated that the ambiguous numerical implementation of substrate limitation could be a serious type of carbon cycle uncertainty, comparable to the uncertainty across the suite of CMIP5 simulations. In particular, such uncertainty may imply the models are simulating (unacknowledged) ecological mechanisms that are inconsistent with the governing equations, which further lead to uncertainties with initial conditions, and ordering of model integrations. Given that more nutrient mechanisms will be introduced in the next generation of land biogeochemical models, this ambiguity will be even more important and potentially a very large source of uncertainty. For a robust numerical coupling of carbon and nutrient dynamics, we suggest modellers should: (1) abandon the law of minimum as an analytically explicit constraint to individual entities in the biogeochemical systems; (2) represent substrate competition in their models with explicit substrate kinetics, (3) use more advanced numerical solvers, and (4) document their model implementations with more technique details. With such, we could thence better understand if we are increasing the model complexity for the right reasons.

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Appendix A. Example misuse of Liebig's law of the minimum

We build our example based on the classic model by Leon and Tumpson (1975), which is

$$\frac{dN_i}{dt}=N_i\left[\min_j\left\{\frac{g_{ij}\left(R_j\right)}{q_{ij}}\right\}-D_i\right],\begin{cases} i=1,\cdots,n \\ j=1,\cdots,n \end{cases} \tag{A-1}$$

$$\frac{dR_i}{dt}=f_j\left(R_j\right)-\sum_i q_{ij}\left[\min_j\left\{\frac{g_{ij}\left(R_j\right)}{q_{ij}}\right\}\right]N_i,\begin{cases} i=1,\cdots,n \\ j=1,\cdots,n \end{cases} \tag{A-2}$$

where N_i is consumer *i* biomass density. R_j is resource *j* (bio)mass density or concentration, or whatever variable is appropriate to the form of the resource. $f_j\left(R_j\right)$ is net supply rate of resource *j*, which could be either positive or negative. $g_{ij}\left(R_j\right)$ is rate of removal of the *j*-th resource by each individual of the *i*-th consumer population. q_{ij} is the conversion factor of units of *j* into units of *i* (or the reciprocal of substrate use efficiency of *j*-th substrate by *i*-th consumer population).

This model describes the growth of a community of populations (denoted by *i*) on a set of perfectly complementary substrates (denoted by *j*) based on Liebig's law of the minimum. However, this application of law of the minimum is incorrect. We back up our assertion with the following explanation.

Suppose there is only one population feeding on two perfectly complementary substrates, then by approximating equations (A-1) and (A-2) with the Euler forward form, we obtain

$$N_1(t+\Delta t)=N_1(t)+\Delta t N_1(t)\left[\min\left\{\frac{g_{11}(R_1(t))}{q_{11}},\frac{g_{12}(R_2(t))}{q_{12}}\right\}-D_1\right] \tag{A-3}$$

$$R_1(t+\Delta t)=R_1(t)+\Delta t f_1(R_1)-\Delta t q_{11}\left[\min_j\left\{\frac{g_{ij}(R_j)}{q_{ij}}\right\}\right]N_1, j=1,2 \tag{A-4}$$

$$R_2(t+\Delta t)=R_2(t)+\Delta t f_2(R_2)-\Delta t q_{12}\left[\min_j\left\{\frac{g_{ij}(R_j)}{q_{ij}}\right\}\right]N_1, j=1,2 \tag{A-5}$$

Now suppose population N_1 is locally limited by substrate R_1, such that $g_{11}(R_1(t))/q_{11}<g_{12}(R_2(t))/q_{12}$, which leads to

$$N_1(t+\Delta t)=N_1(t)+\Delta t N_1(t)\left[\frac{g_{11}(R_1(t))}{q_{11}}-D_1\right] \tag{A-6}$$

$$R_1(t+\Delta t)=R_1(t)+\Delta t\left[f_1(R_1)-g_{11}(R_1)N_1\right] \tag{A-7}$$

$$R_2(t+\Delta t)=R_2(t)+\Delta t\left[f_2(R_2)-\frac{q_{12}}{q_{11}}g_{11}(R_1)N_1\right] \tag{A-8}$$

Now define

$$\lambda=\frac{g_{11}(R_1(t))}{g_{12}(R_2(t))}\frac{q_{12}}{q_{11}} \tag{A-9}$$

Where it can be verified that $\lambda<1$. Then by entering equation (A-9) into (A-8), we obtain

$$R_2(t+\Delta t)=R_2(t)+\Delta t\left[f_2(R_2)-\lambda g_{12}(R_2)N_1\right] \tag{A-10}$$

Now if $R_1\left(t+\Delta t\right)>0$ and $R_2\left(t+\Delta t\right)<0$, both of which can be easily satisfied (note $f_2\left(R_2\right)$ could be negative), then population N_1 is de facto limited by substrate R_2, which is opposite to the "local constraint" that the growth of population N_1 is limited by substrate R_1. Now in order to avoid $R_2\left(t+\Delta t\right)<0$, a numerical substrate limitation must be done, and the use of Liebig's law of minimum in growth rate calculation in equation (A-3) is inappropriate such that it results in a double counting of substrate limitation. For a community of many populations and substrate, we expect such misuse of Liebig's law of minimum could occur even more frequently, and should be avoided.

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Author Contributions

J.Y. Tang designed the study and conducted the experiments. J.Y. Tang and W. J. Riley discussed the results and wrote the paper.

Acknowledgments

This research was supported by the Director, Office of Science, Office of Biological and Environmental Research of the US Department of Energy under contract No. DE-AC02-05CH11231 as part of the Accelerated Climate Model for Energy in the Earth system Modeling program, as well as the Regional and Global Climate Modeling (RGCM) Program. The study used the Lawrencium computational cluster resource provided by the IT Division at the Lawrence Berkeley National Laboratory. The data used in this paper can be obtained by contacting the first author at jinyuntang@lbl.gov.

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Table 1. Model configurations used to evaluate the uncertainty of ambiguous numerical implementation of nutrient limitation.

Simulation ID	Model configuration
MNL	Mineral Nitrogen based Limitation scheme: only existing mineral nitrogen is available for uptake at current time step. It implements equation (3).
NUL	Net nitrogen Uptake based Limitation scheme: mineral nitrogen demand is calculated as the residual between total nitrogen demand and gross mineralization. It implements equation (6).
PNL	Proportional Nitrogen flux based limitation scheme: mineral nitrogen from gross mineralization and existing soil mineral nitrogen are competed equally by plants and microbes. It implements equation (7).
PNLIC	Like PNL, but it uses initial condition from NUL.
PNLO	Like PNL, but O_2 limitation comes after nitrogen limitation. However, a second nitrogen limitation required for avoiding model crash.
Default	ALMv0, which is the de facto CLM4.5BGC.

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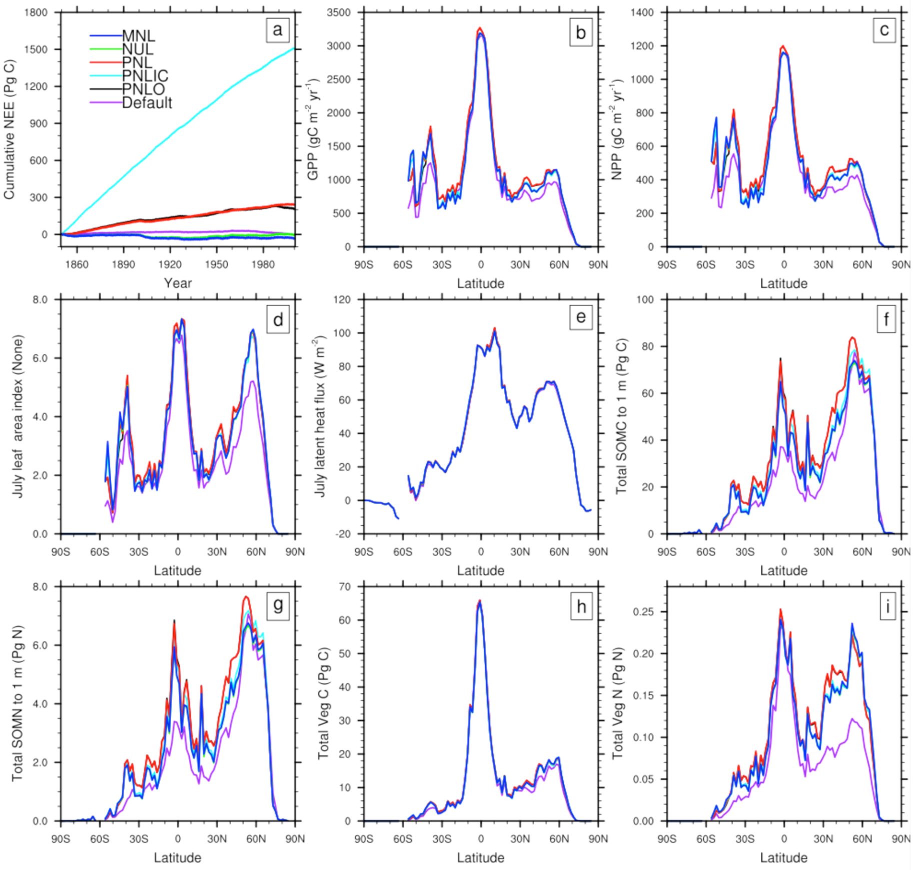

Figure 1. Model predictions for the contemporary period 1850-2000: (a) Cumulative net ecosystem exchange (NEE; positive into the atmosphere); (b) Gross primary productivity; (c) Net primary productivity; (d) July leaf area index; (e) July latent heat flux; (f) total organic soil carbon to 1 m depth; (g) total organic soil nitrogen to 1 m depth; (h) total vegetation carbon; and (i) total vegetation nitrogen. Results for (b)-(i) are averaged over 1991-2000.

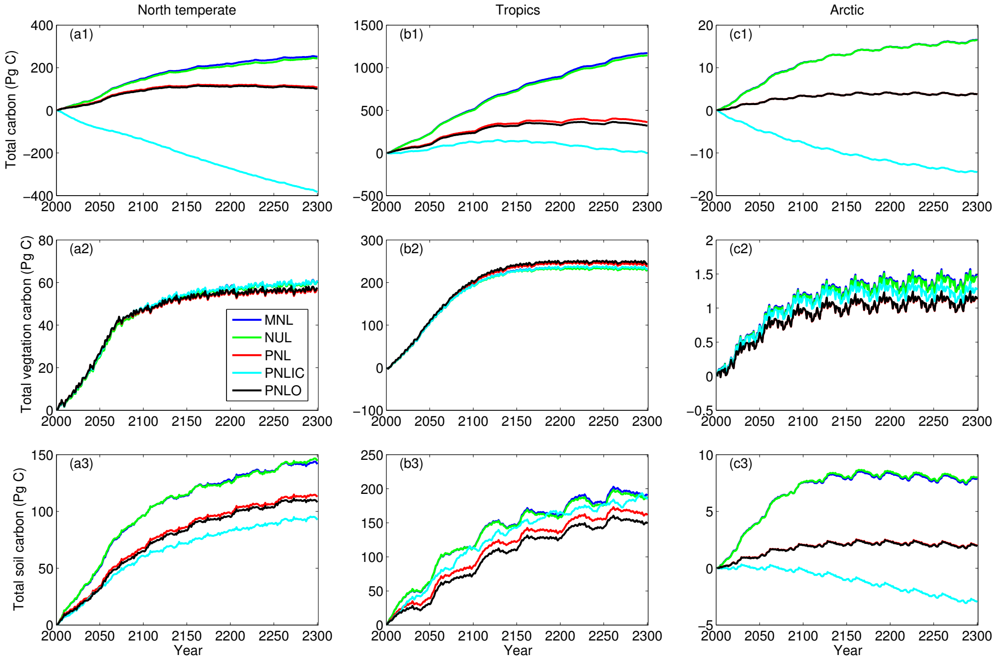

Figure 2. Model simulations forced by the Representative Concentration Pathway 4.5 (RCP4.5) atmospheric CO_2 for year 2001-2300. Here total soil carbon includes litter carbon and soil organic matter as defined in CLM4.5 (Oleson et al., 2013); coarse woody debris is excluded (but can be found in Figure S7). All changes are calculated as relative to each of their initial carbon pool sizes at the start of the simulation (year 2000). The decadal oscillation shown in the figure is due to the cycling of the QIAN climate forcing.

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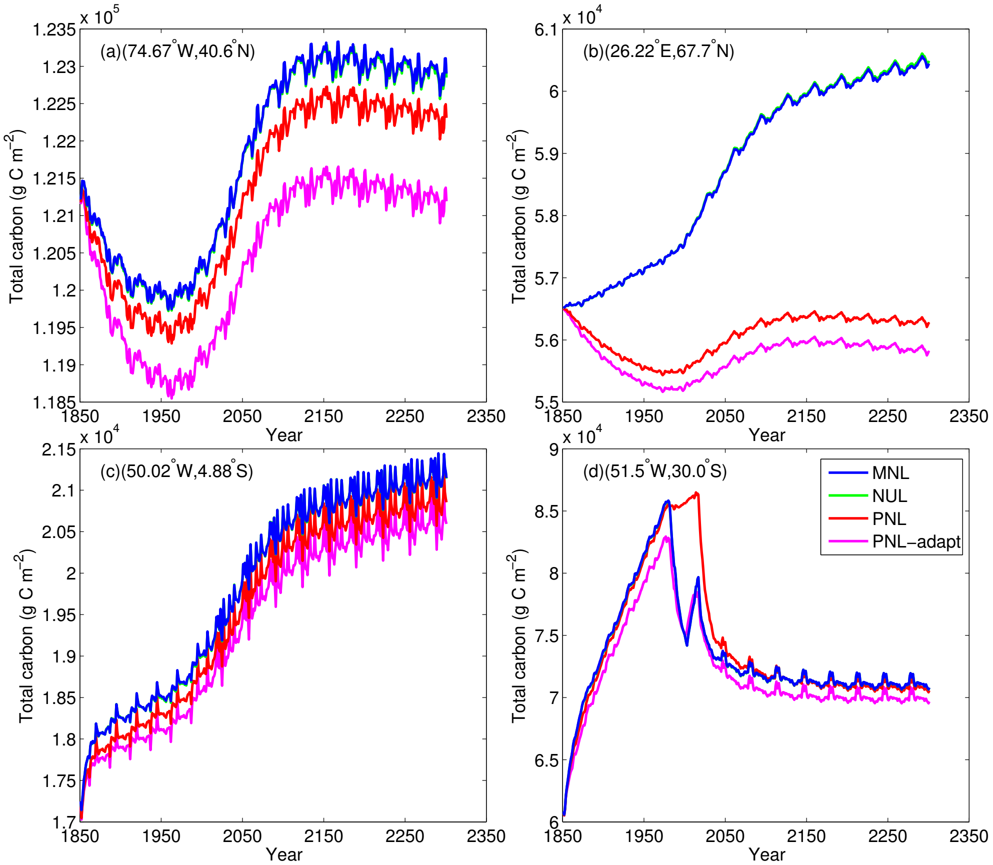

Figure 3. Point simulations for the 4 specific gridcells using different model configratuions. For each site, all simulations used identical initial conditions obtained from spinup with the PNL-adapt code. Note the color schemes are different from that in Figure 1 and Figure 2. The decadal oscillation shown in the figure is due to the cycling of the QIAN climate forcing.

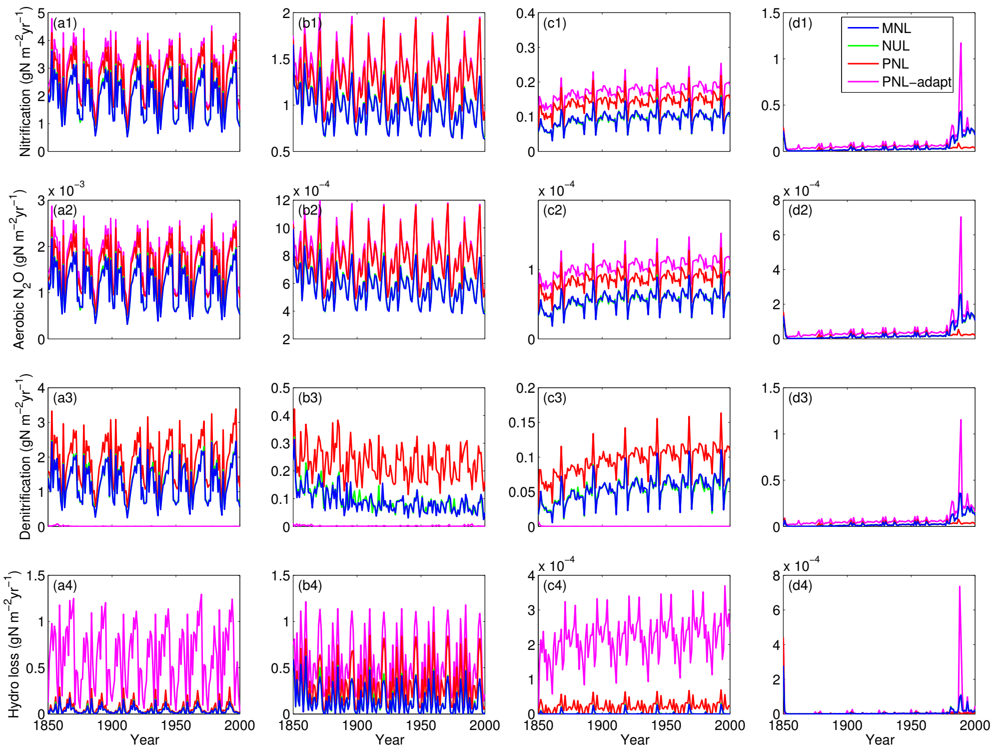

Figure 4. Nitrogen fluxes for the four specific gridcell simulations obtained from different model configurations. The four columns from left to right correspond to the four locations specified in Figure 3. The decadal oscillation shown in the figure is due to the cycling of the QIAN climate forcing.

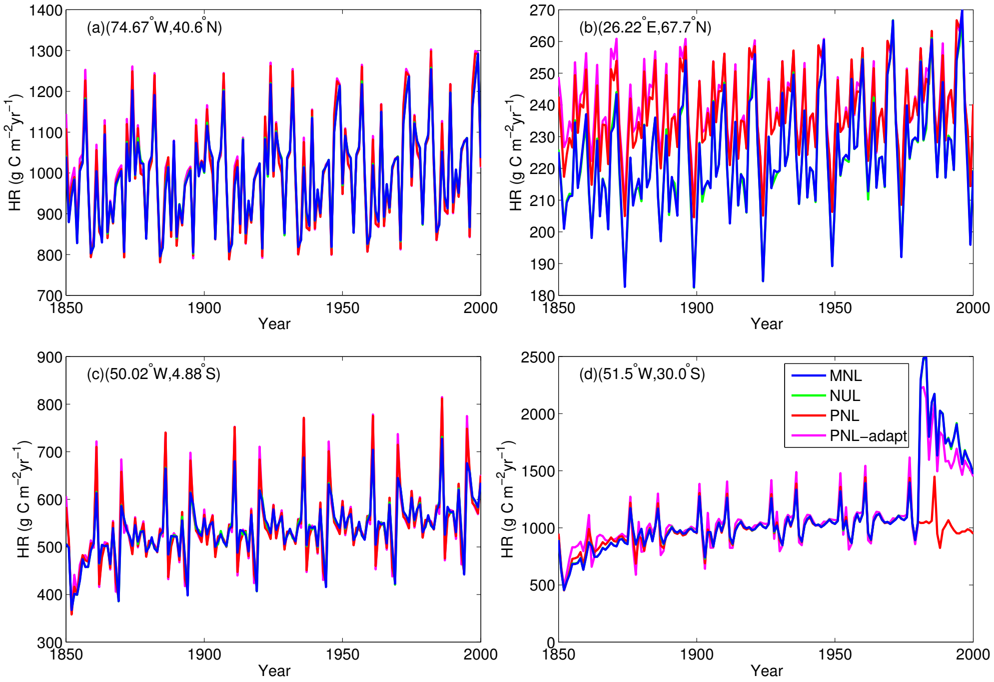

Figure 5. Heterotrophic respiraiton for the four specific gridcell simulations obtained from running different model configurations. The decadal oscillation shown in the figure is due to the cycling of the QIAN climate forcing.

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Supplemental materials for "**Potentially large uncertainty in ecosystem carbon dynamics resulting from ambiguous numerical coupling of carbon and nitrogen biogeochemistry: a demonstration with the ACME land model**"

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1. Introduction of contents

The first part of this supplemental material reports the proof of the sequentially weaker nitrogen limitation in the application of the MNL, NUL and PNL numerical nitrogen limitation schemes. The second part contains figures (**S1-S11**) that provide complementary information to support our results and conclusions in the main text.

2. Proof of the progressively weaker nitrogen limitation

We prove under the same soil mineral nitrogen availability and fluxes of $F_{S,input}$ and $F_{S,uptake}$ that the application of MNL, NUL and PNL schemes leads to progressively weaker nitrogen limitation.

We first prove $\overline{F}_{MNL,uptake} < \overline{F}_{NUL,uptake}$, where, without confusing the readers, the subscript S was removed.

Because substrate S is limited, $\overline{F}_{MNL,uptake} < \overline{F}_{NUL,uptake}$ is equivalent to

$$\frac{S(t)/\Delta t}{F_{S,uptake}} < \frac{S(t)/\Delta t}{F_{S,uptake} - F_{S,input}} \tag{S-1}$$

which is reduced to $F_{S,uptake} - F_{S,input} < F_{S,uptake}$, a condition always holds.

We now prove $\overline{F}_{NUL,uptake} < \overline{F}_{PNL,uptake}$. This requires

$$\frac{S(t)/\Delta t}{F_{S,uptake} - F_{S,input}} < \frac{F_{S,input} + S(t)/\Delta t}{F_{S,uptake}} \tag{S-2}$$

By rearranging the terms of (S-2), we have to show

$$F_{S,uptake}\, S(t)/\Delta t < \left(F_{S,input} + S(t)/\Delta t\right)\left(F_{S,uptake} - F_{S,input}\right) \tag{S-3}$$

which after some rearrangement becomes

$$S(t)/\Delta t < \left(F_{S,uptake} - F_{S,input}\right) \tag{S-4}$$

Since (S-4) is the definition of substrate limitation for the NUL scheme, it always holds under substrate limitation.

We now finish our proof.

List of supplemental figures

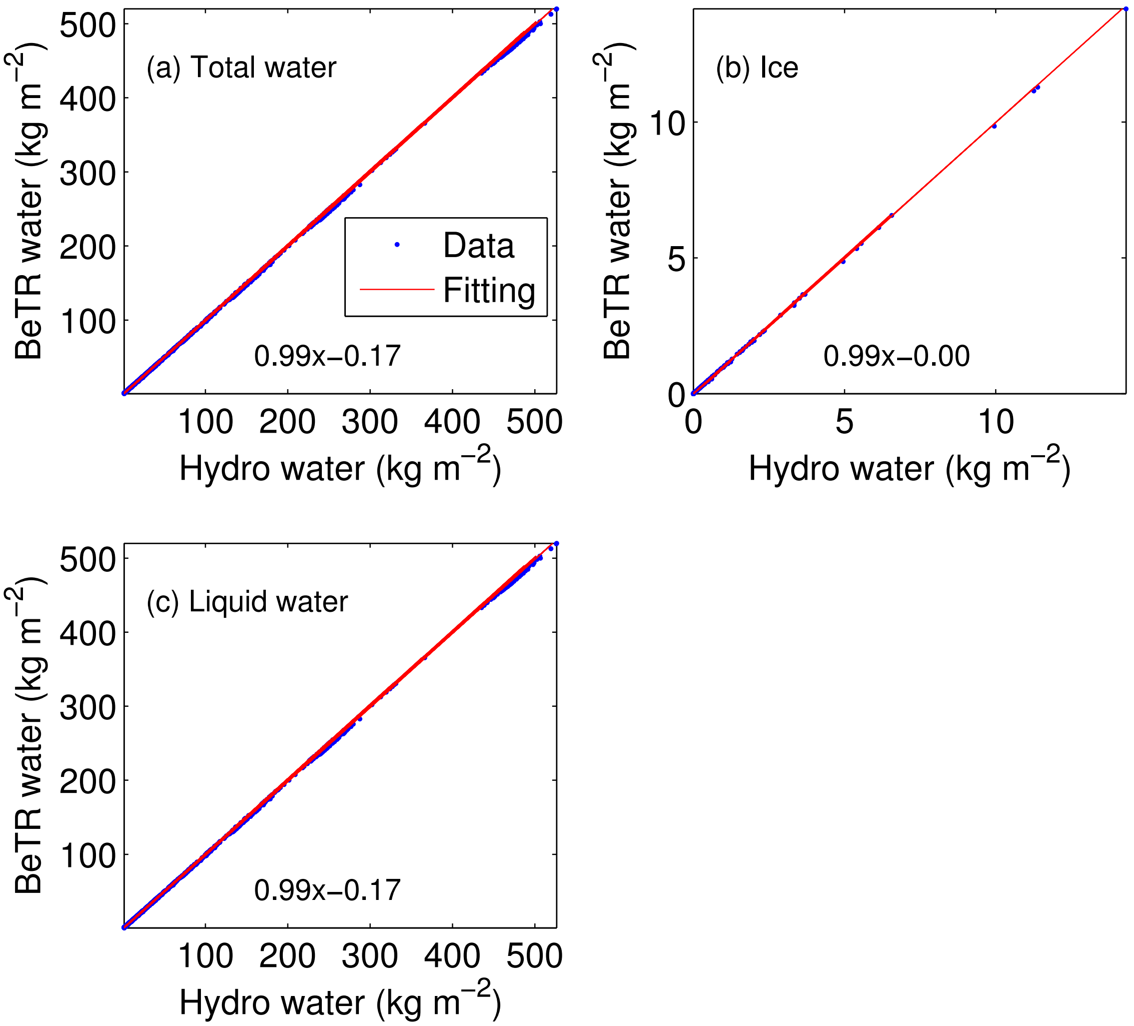

Figure S1. A demonstration of the tracer transport accuracy of BeTR. The Hydro water is water simulated with the biophysics module in the ACME land model. BeTR water is water tracer tracked in BeTR. Ideally, the linear fit should be one to one.

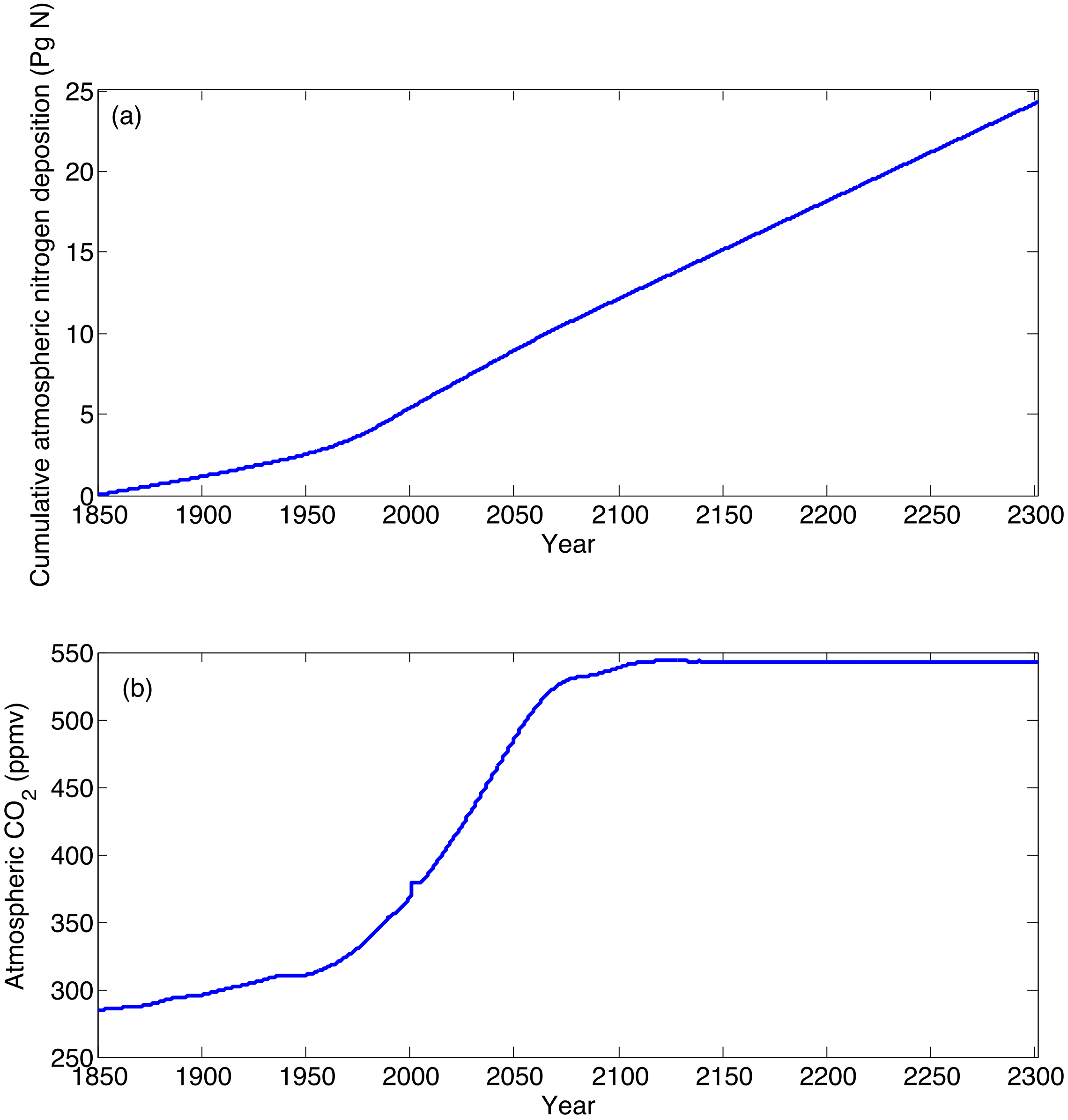

Figure S2: (a) Cumulative atmospheric deposition from 1850 to 2300. (b) Atmospheric CO_2 from 1850 to 2300. The small zigzag in (b) is due to that RCP4.5 CO_2 starts from 2006.

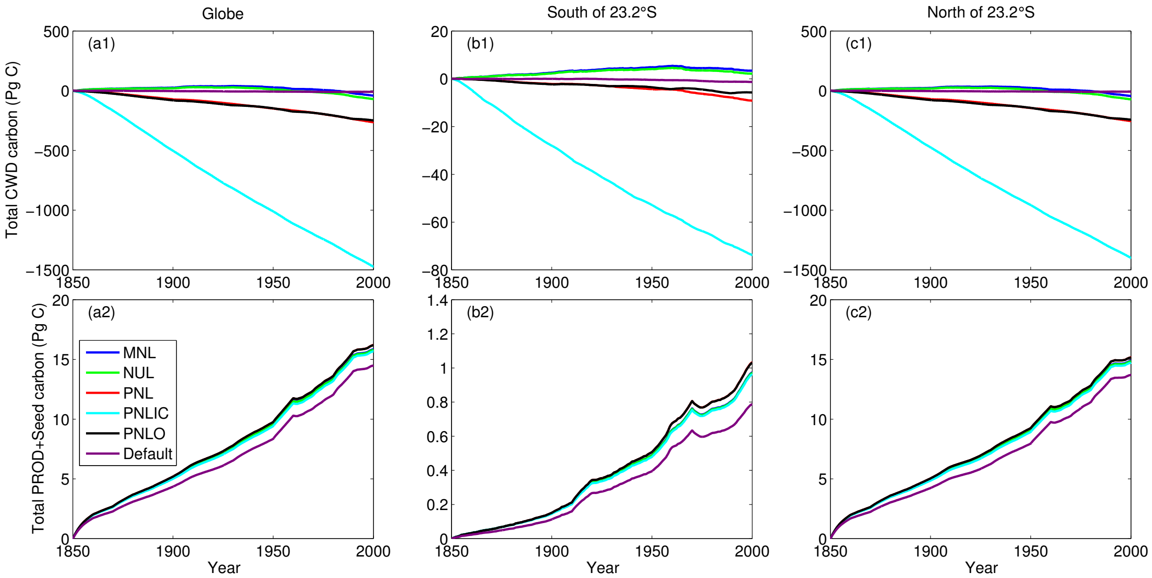

Figure S3: (a1), (b1) and (c1) are carbon changes in total coarse woody debris. (a2), (b2) and (c2) are changes in total product carbon and seed carbon.

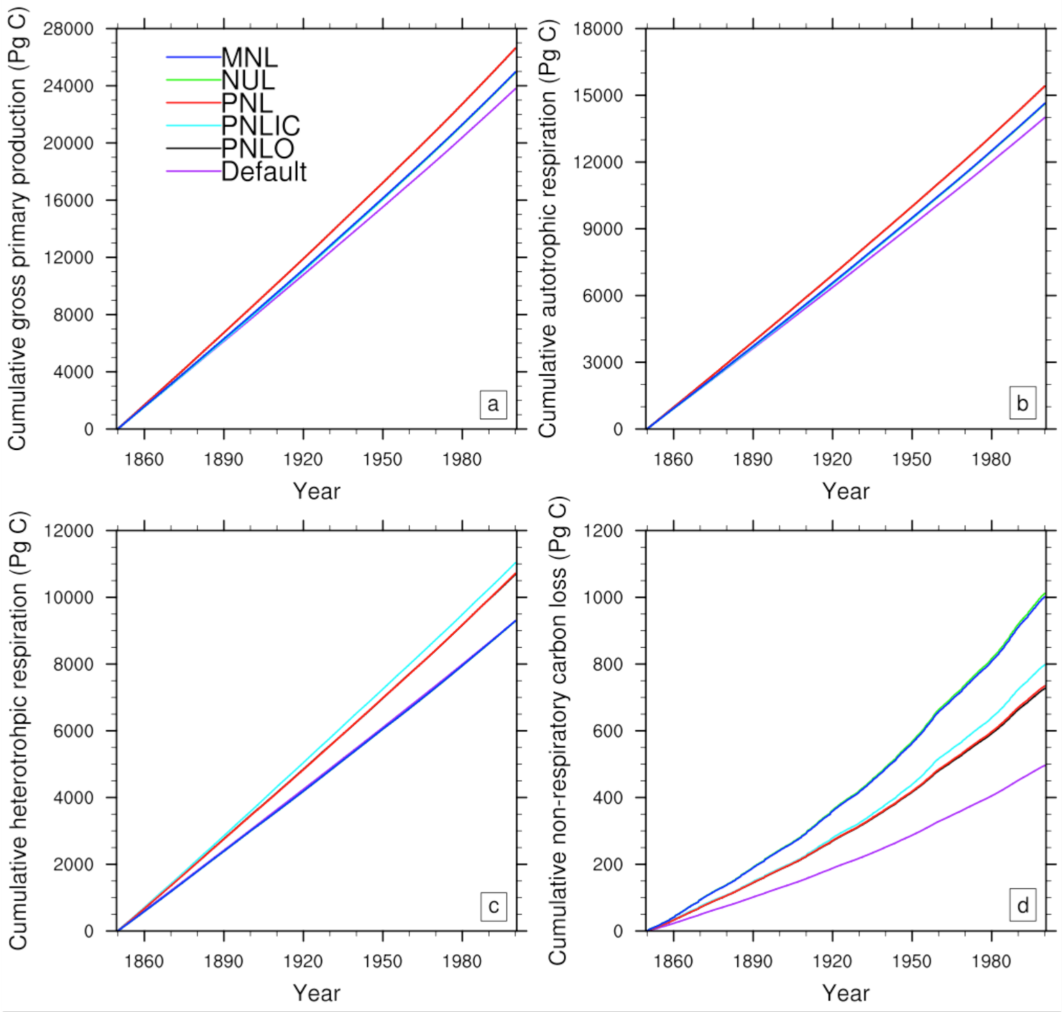

Figure S4. Simulated cumulative carbon fluxes in the contemporary period 1850-2000.

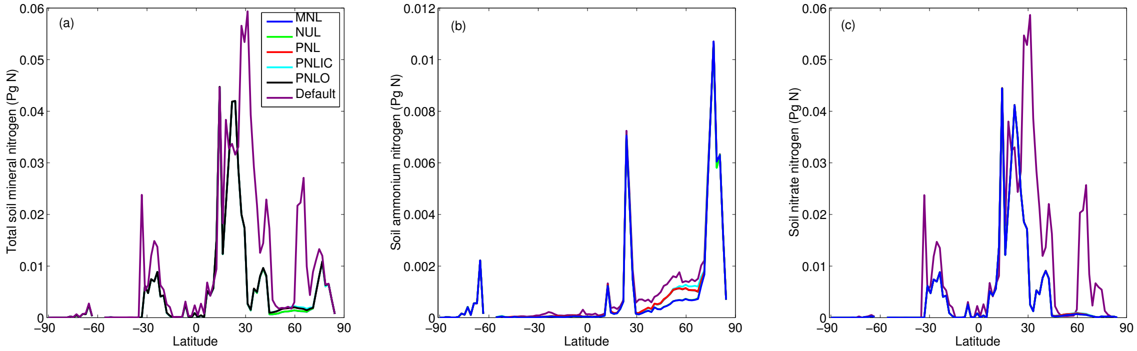

Figure S5: Latitudinal distribution of simulated soil mineral nitrogen for 1991-2000. (a) Total soil mineral nitrogen; (b) NH_4^+ and (c) NO_3^-.

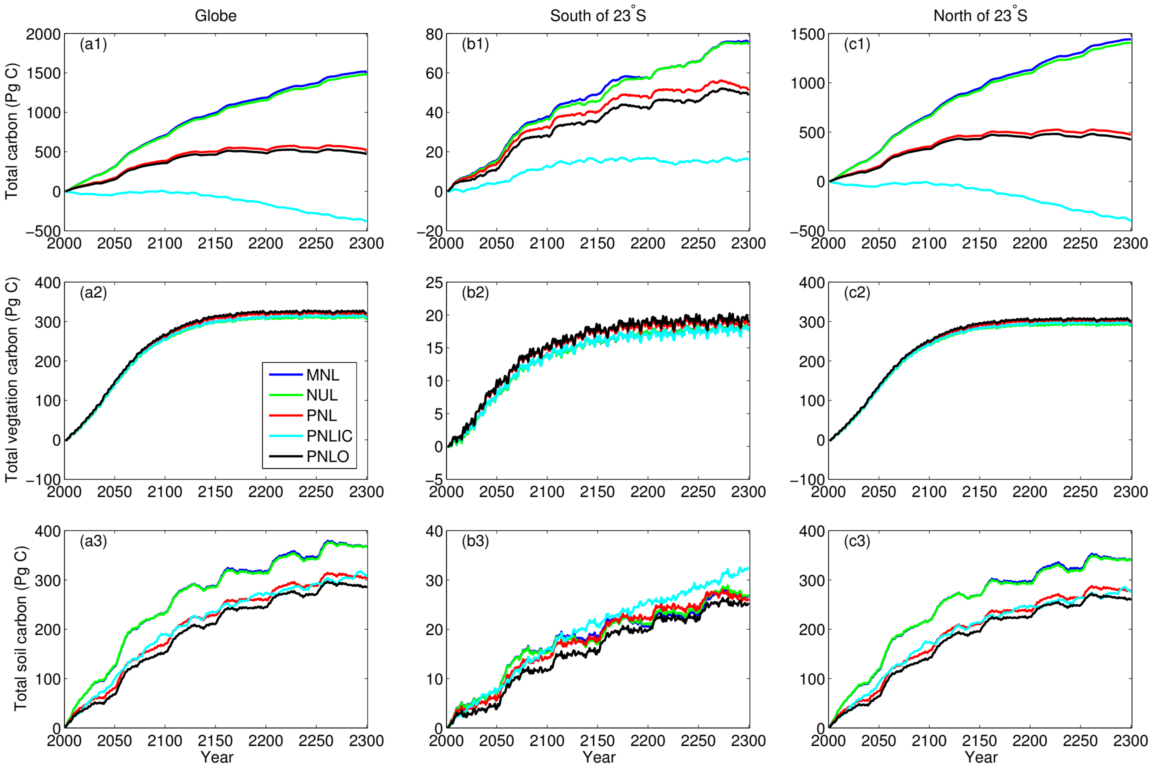

Figure S6: Model simulations for the scenario Representative Concentration Pathway 4.5 (RCP4.5) atmospheric CO_2 for the years 2001-2300. Here total soil carbon includes litter carbon and soil organic matter as defined in CLM4.5; coarse woody debris is excluded. All changes are calculated as relative to each of their initial carbon pool sizes at the start of the simulation (i.e. end of year 2000). The oscillations as shown in the figure are due to the cycling of the QIAN climate forcing.

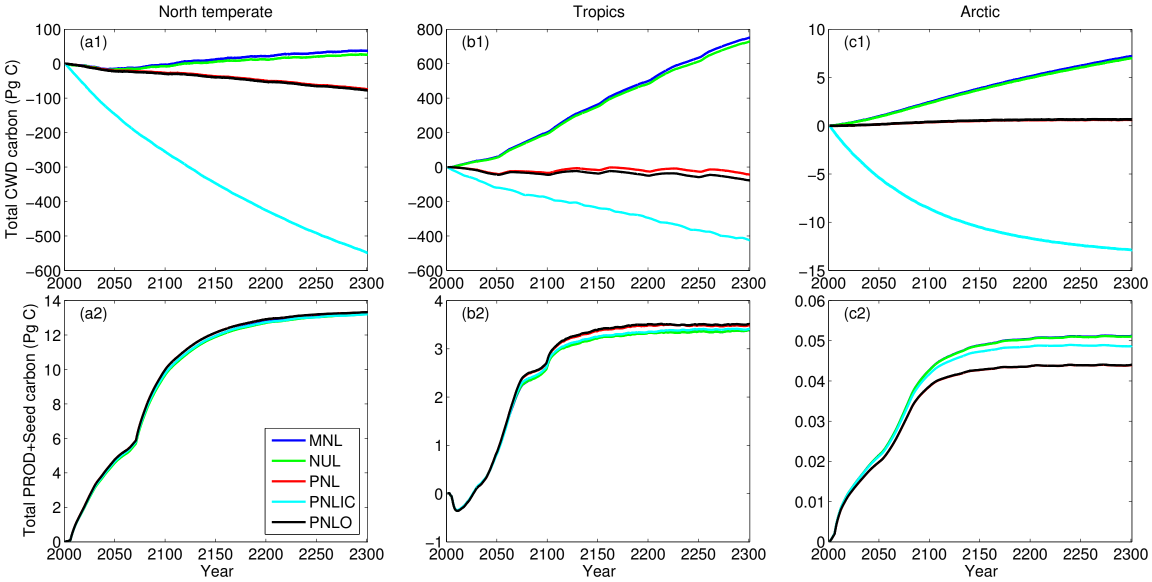

Figure S7: Simulated evolution of coarse woody debris carbon (a1-c1) and product and seed carbon (a2-c2) for the RCP 4.5 CO_2 driven period 2001-2300. These results are complementary to Figure 2 in the main text.

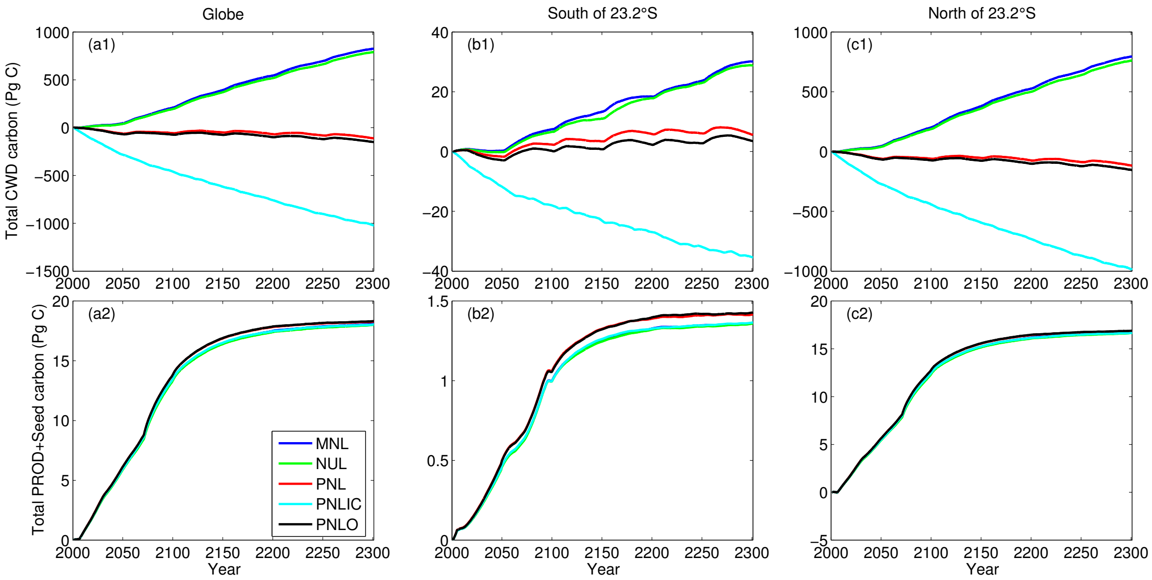

Figure S8: Simulated evolution of coarse woody debris carbon (a1-c1) and product and seed carbon (a2-c2) for the RCP 4.5 CO_2 driven period 2001-2300. These results are complementary to Figure S6 above.

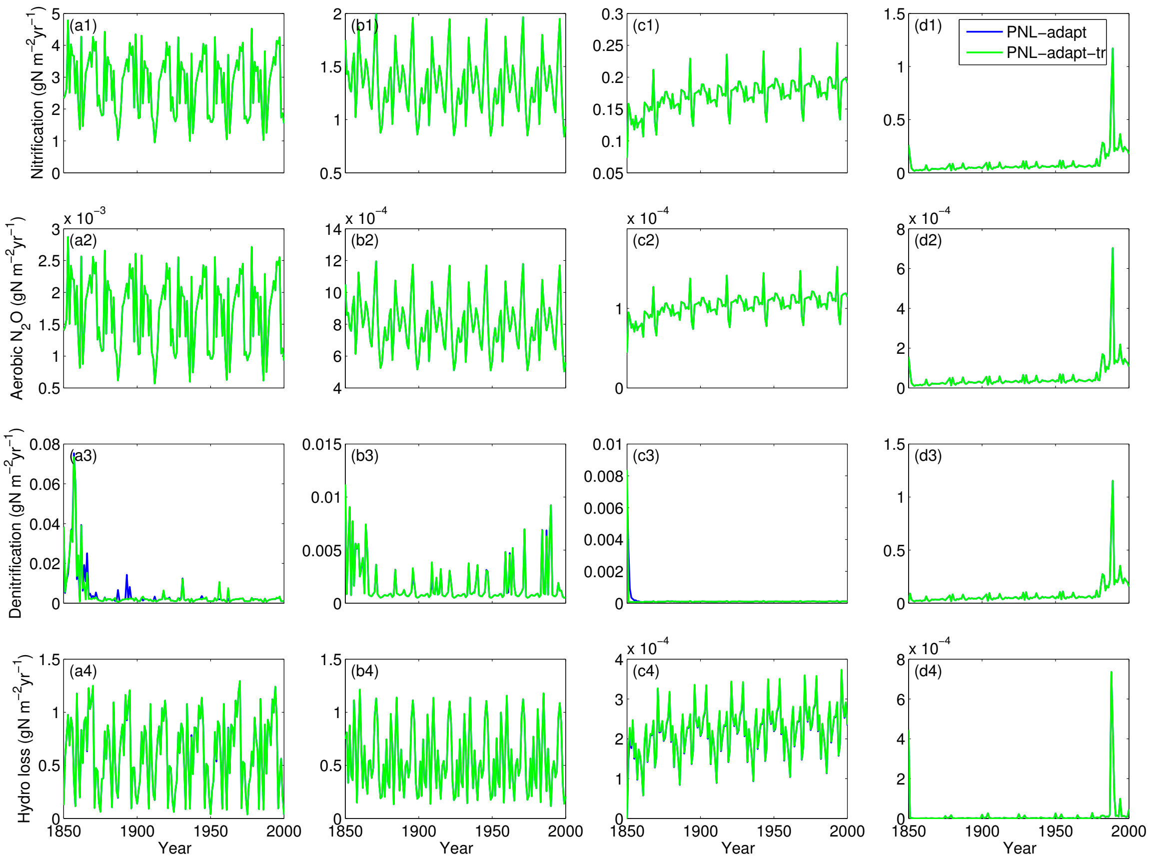

Figure S9: Evaluation of the ordering effect for the point simulations. PNL-adapt-tr simulates transports ahead of biogeochemical calculations, whereas PNL-adapt does the opposite order. From left to right, the four columns are representing sites that are corresponding to the locations specified in Figure 3 of the main text.

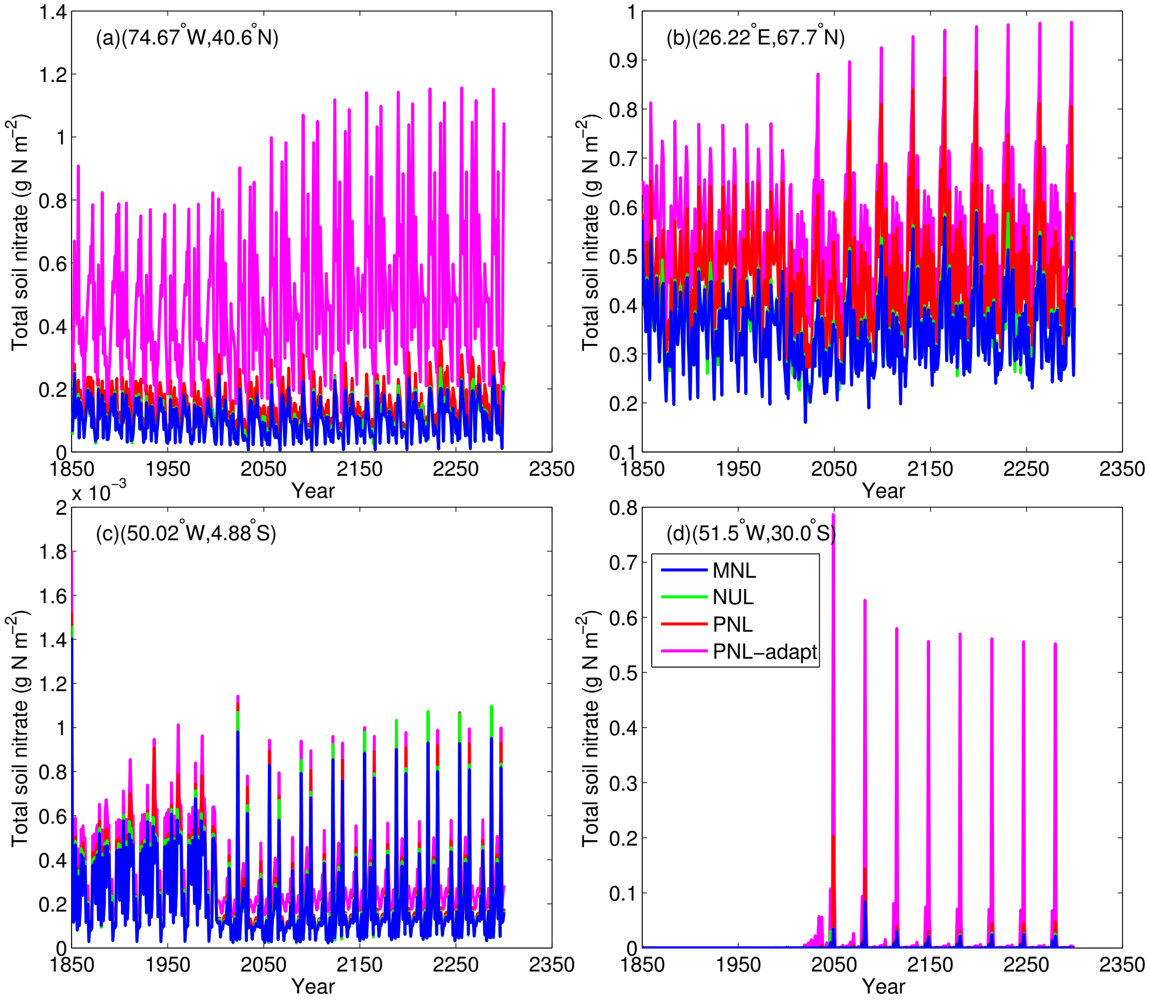

Figure S10: Soil nitrate concentrations for the point simulations as obtained from different model configurations.

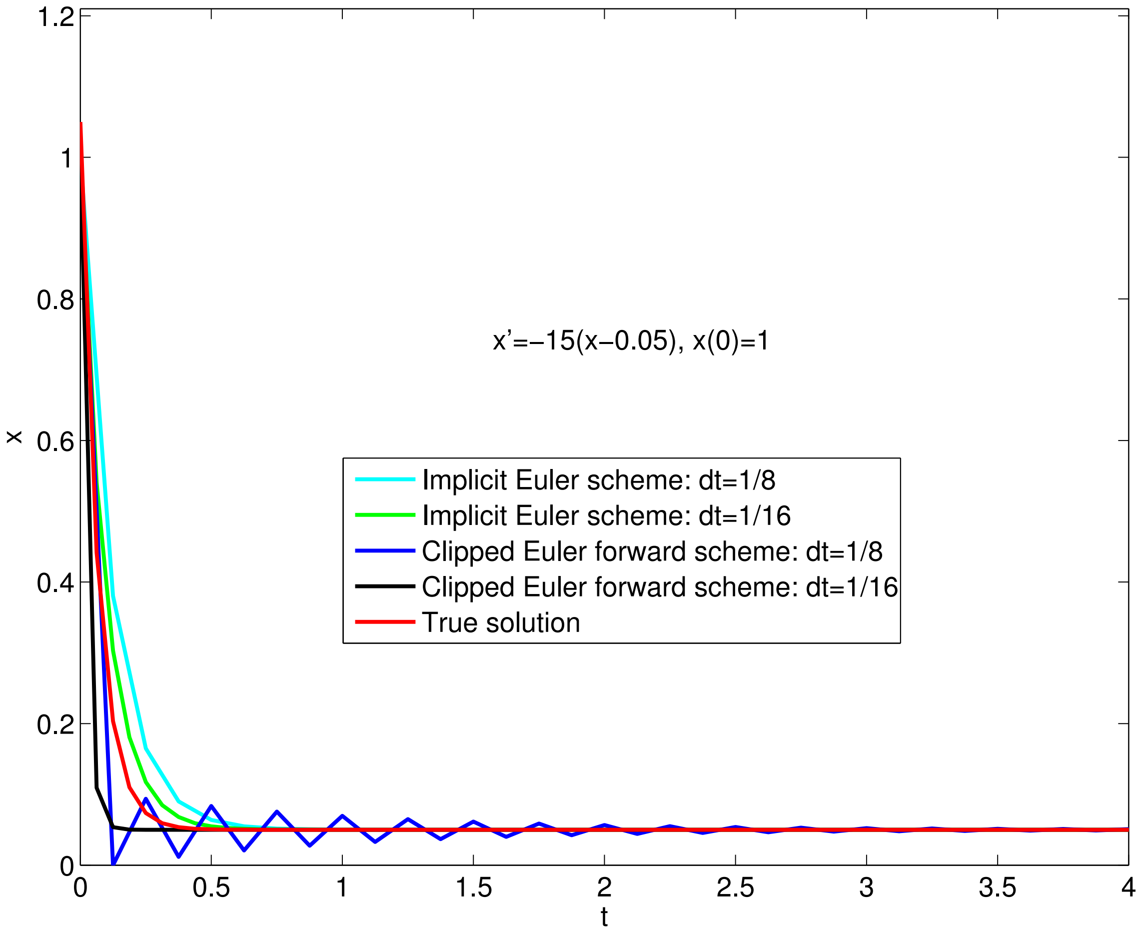

Figure S11: A demonstration of the zigzag phenomena and the strong time-stepping dependence of the numerical solution using Euler methods.