General comments:

Ma et al. describe a new parameterisation for two types of nitrogen fixing crops in tropical and temperate regions for the widely used LPJ-Guess model. They clearly explain and document the added mathematical formulation and parameters, provide a succinct evaluation of the model using suitable data and also provide a global evaluation of the consequences of the model implementation in terms of simulated nitrogen fixation and yields. Overall this is a well written paper, which only requires minor adjustments. The model description is sufficient to understand what has been done and tested, but I want to highlight that the manuscript falls short of making the code accessible to the public. The code availability statement says that the code would be made available for review, but I have not been provided with such a link.

We thank the reviewer for providing constructive feedback and apologize for the inaccessible code during the review process due to the link having expired in mid-October. The new code link via SVN access in Lund university is svn://stormbringer.nateko.lu.se/svn/LPJ-GUESS/tags/_publications/newcrops_bnf_evaluation-gmd-2021-260. In the revision to the manuscript, we address all of the points raised by the reviewer, and we think the resulting study is much improved. Specific revisions and responses to each comment are provided in detail below.

Minor comments:

A few model choices have been made that deviate from previous approaches (e.g. how N fix responds to growth stages, that the cap of NPP investment to N fix is, why is oxygen required for N fixation, which is a process happening in anoxic environments, and why is oxygen availability ignored in the water limitation function). It would be helpful for readers and fellow model developers to better understand the motivation of these choices. In each case, probably one - two sentence explaining the choice would be sufficient.

We thank the reviewer for this suggestion. Brief explanations on main BNF-limiting factors will be added to the revised manuscript, as follows.

For BNF response to growth stage (Sect. 2.3): "Much experimental evidence has indicated that the N fixed by legumes varies widely among crop growth stages, with the largest BNF rate observed between the late vegetative phase and the early seed-filling period (Santachiara et al., 2017; Córdova et al. 2020; Ciampitti et al., 2021). In this study, a specific function, similar to the temperature response function, is thus implemented in the BNF scheme to represent the variation of N fixation with the course of legume life cycle."

For water limitation (Sect. 2.3): "Too little water strongly inhibits BNF due to impacts of drought stress on nodule nitrogenase activity (Serraj et al., 1999; Marino et al., 2007). Although oxygen is needed to support the respiration of legume roots and bacteria in the nodules, nitrogenase is more active in anoxic, waterlogged environments (Jiang et al., 2021). A linear water-limitation function is thus incorporated into LPJ-GUESS (Wu and McGechan, 1999)."

As the reviewer mentions, the implementation of the NPP cost for BNF in our study is different from previous studies. Thus, we would like to give an in-depth discussion in Sect. 4.1: "N fixation can help grain legumes to dramatically enhance their total N accumulation and to achieve higher N concentration in seeds. However, these benefits are accompanied by an increase in respiration cost amounting to 4-16% of fixed total photosynthetic carbon (Kaschuk et al., 2009, 2010). Such a respiratory photosynthate consumption would reduce productivity if photosynthesis rate was not increased to compensate for the cost. In LPJ-GUESS, as described in Sect. 2.3, we assumed that up to 50% of daily NPP can be consumed to fix N. This approach has the advantage that legumes are able to maximize photosynthetic gain due to reduced N limitation in carboxylation capacity (V_{max}), but it entails the risk of lower productivity if too much NPP is invested into fixation. Nevertheless, in most cases our modelled NPP cost over the soybean growing season was ranging from 1-40 % at site scale (Fig. S7) and 5-25% on a large region (Fig. S8). Such NPP consumption was not only lower than our assumed upper limit of 50%, but also appropriately consistent with the reported

range of 14-32% described by Kaschuk et al. (2009), demonstrating that the C cost scheme implemented for N fixation in our model is reasonable."

A somewhat more comprehensive explanation on the calculation of planting dates would be appreciated.

We agree with the reviewer's opinion that a comprehensive description on the representation of sowing dates would be helpful for readers to understand the crop growth in the model. Generally, LPJ-GUESS adopts the dynamic sowing dates based on local climate with five seasonality types incorporated (Waha et al., 2012). The five seasonality types are determined by temperature and precipitation conditions, with the intra-annual variability of temperature and precipitation being especially important. We applied specific rules per seasonality type to simulate sowing date. For example, in the region with temperature seasonality, sowing starts when daily average temperature exceeds a prescribed crop-specific threshold. In the region with precipitation seasonality, we assumed that crops sow at the onset of the main rainy season, which in the model is defined as the largest sum of monthly precipitation-to-potential-evapotranspiration ratios of four consecutive months (Lindeskog et al., 2013). More details can refer to the description in Waha et al. (2012).

We will add a brief explanation of crop growth periods in Sect. 2.1 in the new manuscript. Suggested revision: "Sowing dates on a large scale are determined dynamically in the model based on local climatology in each grid cell with five seasonality types represented (combination of temperature and precipitation limited behaviors, Waha et al., 2012), and crops are harvested once each year when prescribed heat sum requirements are fulfilled (Lindeskog et al., 2013). "

The method description is not explicit about the source of N fertiliser used. This information should be added to Section 2.4. It is specifically important to clarify how the authors have dealt with the N fertiliser information that is related to cropland N fixation, which is included as a factor in many estimates of N fertiliser application.

Globally, time-dependent mineral N fertilizer and manure used in this study are taken from Ag-GRID (AgMIP GRIDded Crop Modeling Initiative; Elliott et al. (2015) and Zhang et al. (2017), respectively). The application rates of these two N fertilizer types to soybean and pulses are given in the figure below, averaged over the period of 1996-2005 (kg N ha⁻¹). The figure will be added to the SI of the revised manuscript.



Figure S4. Global map of mineral N fertilizer (a) and total fertilizer inputs (mineral N + manure) (b) for soybean (top) and pulses (bottom), averaged over 1996-2005 (kg N ha⁻¹, see Sect. 2.4.2).

We also add the N fertilizer information in Sect. 2.4.2 as suggested, including the timing and amount of application, as well as the fertilizer sources. Suggested revision: "In terms of timing of N fertilizer application, a recent meta-analysis conducted by Mourtzinis et al. (2018) indicated that splitting N application between planting and the early reproductive stage resulted in significantly greater soybean yields than a single application. Mineral N fertilizer for legumes was thus split into two equal applications at the time of sowing (DS=0) and flowering (DS=1.0). Manure was added to soils at the time of sowing as a single application to reflect real-world practices that account for the time required for manure N to be made available to plants. Data sources for mineral N fertilizer and manure over the period 1901-2014 were derived from Ag-GRID (AgMIP GRIDded Crop Modeling Initiative; Elliott et al. (2015) and Zhang et al. (2017), respectively) (Fig.S4)."

Figure 4: Please be specific, which regression data belongs to which simulation set.

To make it clearer to readers, we will update the legend of Figure 4 and add the relevant explanations on linear regression in caption.

Suggested revision for the caption of figure 4: "Comparison of modelled and observed yield (a), grain N mass (b), shoot N mass (c), soil N uptake (d), BNF (e) and %Ndfa (the proportion of plant N derived from the atmosphere) (f) at harvest across all soybean and faba bean sites. Filled red and grey circles depict the 'site-specific' and 'global-uniform' runs, respectively. The dashed line is fitted linear regression with red for 'site-specific' and grey for 'global-uniform'; *** and ** denote regressions statistically significant at p=0.001 and 0.01, respectively; AB is absolute bias (Eq. 17), represented in percent (%); the unit of RMSE is the same as the associated variable; AVG in (f) is the averaged value of %Ndfa across all field trials".

Figure 6: does panel e not suggest that there's something wrong in the time dependence of N fixation?

In the real world, it might take a while after inoculation for nodulation to happen and fixation to reach full capacity, but in LPJ-GUESS we assume that all the fixation machinery is there and ready to work after a few days of planting (see Eq.12). Another possible explanation is the difference between the simulated and observed crop growing stage at this Austrian soybean site, mainly due to the use of GSWP3-W5E5 climate data set in our simulation (see Sect. 2.4.1, because of the unavailability of field-based weather records at majority of sites evaluated). The daily mean temperature from this reanalysis data set is most likely differing from the field observations because the grid cell at 0.5° coarse resolution in GSWP3-W5E5 may not realistically represent the field-based weather conditions on the fine scale (see Figure below, we compared the climate difference between GSWP3-W5E5 and field-based records at three sites). The temperature difference would affect the legume development stage via accumulated heat units (see Eq.1), and subsequently bias the daily pattern of N fixation in the model. However, from the perspective of the entire growing season, our modelled total N fixation is close to the measured value at harvest (see Table 2).



Figure S2. Comparison of daily climate between GSWP3-W5E5 data set and field-based weather records over the experimental period at USA-Illinois (a), Spain-Lugo (b), and Kenya- Kisumu sites (c). RB and AB are mean relative bias (Eq. 16) and absolute bias (Eq. 17), respectively, presented in percent (%). See Table S2 for the BNF trials of these three sites.

Figure 9: Please attempt to arrange the panels more logically (e.g. placement of China and Canada?).

We arranged the panels of top 10 soybean-producing countries (i.e., b-k) based on their total production from 1996-2005. For example, the largest production country (U.S.A.) is labeled as (b), the second largest producer (Brazil) is labeled as (c), etc. To make it clearer to readers, we add the explanations in the figure caption.

Suggested revision: "Comparison of simulated and FAO-reported yields on country level averaged over 1996–2005 (a), as well as time series of modelled soybean yield (red solid line) and reported FAO statistics (black dashed line) in the top 10 producer countries over the period 1981–2016. The top 10 producer countries (b–k, in descending order) were chosen based on their total production from 1996–2005. *r* is Pearson correlation coefficient (Eq. 19), where ***, ** and * denote the correlation to be statistically significant at p=0.001, 0.01, and 0.05 level, respectively. RB is relative bias (Eq. 16), represented in percent (%). SD_{Rep} and SD_{Mod} denote, respectively, reported and modelled yield standard deviations (t ha⁻¹ yr⁻¹) from 1981-2016".

Figure 10: Here it is important to understand what the underlying N fertilisation data source was, and to which extend this contributes to finding?

As explained above, a global map of N fertilizer inputs will be added to the SI of the revised manuscript, and data source information will be added to Sect. 2.4.2 as suggested, including the timing and amount of application. We agree with the reviewer opinion that N fertilizer could affect the modelled N fixation rate regionally. For instance, the low simulated soybean %Ndfa (the proportion of plant N derived from the atmosphere) in East Asia may reflect high N uptake from soils in response to substantial fertilizer investment in China (80-180 kg N ha⁻¹ yr⁻¹, see the N fertilizer map above). In contrast, the high modelled %Ndfa in Africa was found in our simulations. We will revise the relevant sentences in the main text to highlight the contribution of N fertilizer to our findings.

Suggested revision in Sect. 3.2.2: "Moreover, the relatively low fertilizer application in Africa (0-20 kg N ha⁻¹ yr⁻¹, Fig. S4b) leaves a nitrogen deficit that causes enhanced soybean N fixation. In contrast, in arid and semi-arid regions, soil water constrains BNF, while temperature limitation is seen in high latitudes and alpine areas (e.g., Andes in Peru). BNF rates in most regions (South Asia, West Asia, Sub-Saharan Africa and northwest China) were as low as 50 kg N ha⁻¹ yr⁻¹, particularly in Pakistan and northern India, where simulated BNF is severely constrained by the extreme high temperature over the cropping season. Eastern United States, Europe, Southern China and central-west Brazil showed intermediate fixation rates, which were greater than 150 kg N ha⁻¹ yr⁻¹. Overall, the spatial variation of modelled legume BNF rate reflects to large degree the spatial climate patterns, in addition to N-fertilizer application. The low modelled %Ndfa of $45\pm3\%$ in East Asia may reflect high N uptake from soils in response to substantial fertilizer investment in China (80-180 kg N ha⁻¹ yr⁻¹, Fig. S4b) over the past 40 years. In contrast, the modelled %Ndfa in Africa—with lower N application rates—was as high as $70\pm3\%$, although still lower than the reported mean value of 77% (Table 3)".

References

Ciampitti, I. A., de Borja Reis, A. F., Córdova, S. C., Castellano, M. J., Archontoulis, S. V., Correndo, A. A., Antunes De Almeida, L. F. and Moro Rosso, L. H.: Revisiting Biological Nitrogen Fixation Dynamics in Soybeans, Front. Plant Sci., 12(October), 1–11, doi:10.3389/fpls.2021.727021, 2021.

Córdova, S. C., Archontoulis, S. V. and Licht, M. A.: Soybean profitability and yield component response to nitrogen fertilizer in Iowa, Agrosystems, Geosci. Environ., 3(1), 1–16, doi:10.1002/agg2.20092, 2020.

Elliott, J., Müller, C., Deryng, D., Chryssanthacopoulos, J., Boote, K. J., Büchner, M., Foster, I., Glotter, M., Heinke, J., Iizumi, T., Izaurralde, R. C., Mueller, N. D., Ray, D. K., Rosenzweig, C., Ruane, A. C. and Sheffield, J.: The Global Gridded Crop Model Intercomparison: Data and modeling protocols for Phase 1 (v1.0), Geosci. Model Dev., 8(2), 261–277, doi:10.5194/gmd-8-261-2015, 2015.

Jiang, S., Jardinaud, M., Gao, J., Pecrix, Y., Wen, J., Mysore, K., Xu, P., Sanchez-canizares, C., Ruan, Y., Li, Q., Zhu, M., Li, F., Wang, E., Poole, P. S., Gamas, P. and Murray, J. D.: NIN-like protein transcription factors regulate leghemoglobin genes in legume nodules, Science (80-.)., 374, 625–628, 2021.

Kaschuk, G., Kuyper, T. W., Leffelaar, P. A., Hungria, M. and Giller, K. E.: Are the rates of photosynthesis stimulated by the carbon sink strength of rhizobial and arbuscular mycorrhizal symbioses?, Soil Biol. Biochem., 41(6), 1233–1244, doi:10.1016/j.soilbio.2009.03.005, 2009.

Kaschuk, G., Hungria, M., Leffelaar, P. A., Giller, K. E. and Kuyper, T. W.: Differences in photosynthetic behaviour and leaf senescence of soybean (Glycine max [L.] Merrill) dependent on N2 fixation or nitrate supply, Plant Biol., 12(1), 60–69, doi:10.1111/j.1438-8677.2009.00211.x, 2010.

Lindeskog, M., Arneth, A., Bondeau, A., Waha, K., Seaquist, J., Olin, S. and Smith, B.: Implications of accounting for land use in simulations of ecosystem carbon cycling in Africa, Earth Syst. Dyn., 4(2), 385–407, doi:10.5194/esd-4-385-2013, 2013.

Marino, D., Frendo, P., Ladrera, R., Zabalza, A., Puppo, A., Arrese-Igor, C. and Gonzalez, E. M.: Nitrogen Fixation Control under Drought Stress. Localized or Systemic?, Plant Physiol., 143(4), 1968–1974, doi:10.1104/pp.106.097139, 2007.

Mourtzinis, S., Kaur, G., Orlowski, J. M., Shapiro, C. A., Lee, C. D., Wortmann, C., Holshouser, D., Nafziger, E. D., Kandel, H., Niekamp, J., Ross, W. J., Lofton, J., Vonk, J., Roozeboom, K. L., Thelen, K. D., Lindsey, L. E., Staton, M., Naeve, S. L., Casteel, S. N., Wiebold, W. J. and Conley, S. P.: Soybean response to nitrogen application across the United States: A synthesis-analysis, F. Crop. Res., 215, 74–82, doi:10.1016/j.fcr.2017.09.035, 2018.

Santachiara, G., Borrás, L. and Rotundo, J. L.: Physiological processes leading to similar yield in contrasting soybean maturity groups, Agron. J., 109(1), 158–167, doi:10.2134/agronj2016.04.0198, 2017.

Serraj, R., Sinclair, T. R. and Purcell, L. C.: Symbiotic N2 fixation response to drought, J. Exp. Bot., 50(331), 143–155, doi:10.1093/jxb/50.331.143, 1999.

Waha, K., Van Bussel, L. G. J., Müller, C. and Bondeau, A.: Climate-driven simulation of global crop sowing dates, Glob. Ecol. Biogeogr., 21(2), 247–259, doi:10.1111/j.1466-8238.2011.00678.x, 2012.

Wu, L. and McGechan, M. B.: Simulation of nitrogen uptake, fixation and leaching in a grass/white clover mixture, Grass Forage Sci., 54(1), 30–41, doi:10.1046/j.1365-2494.1999.00145.x, 1999.

Zhang, B., Tian, H., Lu, C., Dangal, S., Yang, J. and Pan, S.: Manure nitrogen production and application in cropland and rangeland during 1860–2014: A 5-minute gridded global data set for Earth system modeling, Earth Syst. Sci. Data, 9, 667–678, doi:10.5194/essd-2017-11, 2017.