In this work, the authors introduced, in the software MAGEMin (Riel et al., 2022), a more efficient formulation to compute the Gibbs free energy minimization based on the thermodynamic database of Holland et al., (2018). The previous formulation implemented in MAGEMin solved the minimization problem by imposing inequality constraints to bound the fraction of elements in a given crystallographic site between 0 and 1. This formulation is computationally expensive, because it has to be repeated for all the mixing elements in each crystallographic site of the solid solution, thus taking 75-90 % of the total computation time. Moreover, the minimization can occasionally fail due to violations of the inequality constraints, leading to a poor success rate of 57-97 %. The low performances of the inequality constraints formulation, hinders the coupling of phase equilibria calculation with geodynamic models (e.g., self-consistent reactive fluid transport models). The new formulation introduced in MAGEMin by the authors employs the nullspace approach ($Ax = 0$) to transform the non-linear inequality constraints into a set of linear equalities, which are subsequently turned into a bound-constrained optimization problem: min $f(x)$, with $x > 0$. This formulation can be solved using gradient-based algorithms, which are computationally efficient. While the nullspace approach is not novel, the authors have further compared the performances of four Gibbs free energy minimization algorithms: two with inequality constraints (CCSAQ and SLSQP), and two with bound-constrained optimization methods (CG and BFGS). Here the authors show that the bound-constrained formulation combined with the BFGS algorithm yields the best performance by significantly reducing the minimization time regardless of the dimensionality of the phase model (i.e. the number of oxides used to define the solid solution), while also maintaining a 100% success rate.

This work remarks the efficiency of the bound-constrained optimization method in computing Gibbs free energy minimization compared to inequality constraints formulations. The algorithm described in this paper represents a valuable computational tool, which can be implemented in other phase equilibria calculators. I believe that the bound-constrained formulation is relevant for the broad geodynamic community, as it will allow more efficient coupling between petrological and thermomechanical models. The quality of the manuscript is good, but some minor revisions are needed before its publication.

Line 19: The acronym ‘BFGS’ in the abstract should be explained before its first use.

Line 21: In the conclusions (line 330) you report that the new approach improves the computational time by a factor of ≥ 3; here in the abstract, instead, you report a factor of ≥ 5. Which one is the correct factor?

Lines 28-30: there is an extra bracket between 'MELTS and Connolly'.

Line 37: the notation 10s 100s is misleading, as it can be read as 10 or 100 seconds. It is better to use the order of magnitude, i.e. 10^1, 10^2 milliseconds.

Line 39: same as before line 37; it is better to use the order of magnitude.

Line 59: The acronym ‘CCSAQ’ should be explained before its first use.

Line 62: GeoPS starts with a capital G. Moreover, it is better to start the sentence introducing what GeoPS is, e.g., “The phase equilibria calculator GeoPS...”.

Line 76: does *xeos* mean 'compositional equation of state'? The definition of this term is not intuitive, and it should be explicitly defined in the text.

Line 83: here the symbol and the unit of Gibbs energy is missing, i.e. G_λ and [J].

Line 85: does $p_{i(\lambda)}$ represents the mole fraction [mol]? Otherwise, the unit of measurements of Gibbs energy [J] in equation (1) is not consistent.

Line 86: the unit of measurements of molar chemical potential $\mu_{i(\lambda)}$ [J mol^{-1}] is missing.

Line 90: **"**the *molar* chemical potential of a phase is..." (here molar is missing).

Line 94-95: the unit of measurements of the ideal activity $a^{\mathrm{id}}{}_{i(\lambda)}$, the reference Gibbs energy $\mathrm{g}^{0}{}_{i(\lambda)}$ and the excess energy $\mathrm{g}^{\mathrm{ex}}{}_{i(\lambda)}$ are missing. It should explicitly mention that $a^{\mathrm{id}}{}_{i(\lambda)}$ is dimensionless [/]. To satisfy the dimensional consistency of the equation (2), the two energies $\mathrm{g}^{0}{}_{i(\lambda)}$ and $\mathrm{g}^{\mathrm{ex}}{}_{i(\lambda)}$ should be [J mol^{-1}]. If this is the case, they should be named: reference molar Gibbs energy and excess molar energy.

Equation 4, line 101: why is N_λ now referred to olivine (N_{ol})? This has not been established in the text. N_{ol} is also presented in the summation in line 102. The parameters ϕ'_n and ϕ_n are not described, whereas ϕ_i does not appear in the equation.

Line 102: can you explain what the asymmetry parameter v_i is?

Line 104: the unit of measurements of interaction energy $W_{m,n}$ is missing. It should be [J mol^{-1}].

Equation 5, line 108: there is too much distance between the introduction of the variable x_{cv} (line 114) and its usage in equation 5 (line 108). What does the subscript _cv stand for? composition (c) and order (v)? This parameter should be introduced before equation 5, e.g.: "Given this formulation, the set of equations 1 to 4 can be directly transformed into the following Gibbs free energy minimization problem as a function of the compositional (c) and order (v) variables x_{cv}".

Line 109: here you should explicitly introduce the first inequality constrain, i.e. the fraction of the element $\mathrm{X} \geq 0$.

Line 111: here you should explicitly introduce the second inequality constrain, i.e. the compositional and order variables must be within an upper ($\mathrm{ub}_{\mathrm{cv}}$) and a lower ($\mathrm{lb}_{\mathrm{cv}}$) limit.

Paragraph 118-126: Here the authors should make clear to the reader that they are implementing this new formulation in the code MAGEMin based on the thermodynamic database of Holland et al., (2018). Moreover, the authors should report some literature to remark that the introduction of the nullspace approach is not a novel and it has already been used to computed the Gibbs free energy minimization in other phase equilibria calculators (e.g., HeFESTo Stixrude and Lithgow-Bertelloni, 2011 - https://doi.org/10.1111/j.1365-246X.2010.04890.x).

Line 120: It is better to avoid having nested brackets e.g., "... crystallographic sites i.e., Bragg–Williams-type formulation (Myhill and Connolly, 2021)".

Lines 122-123: too many consecutive adverbs (numerically, significantly, costly). Try with: "which has a significantly higher numerical cost compared to the bound-constrained minimization algorithms".

Line 131: the sentence in the bracket can be moved after the equations e.g., "Note that we have dropped the ion charges in the notation of the equations".

Equation 17, line 155: It would be clearer to the reader to define x = X_{es} already here.

Equation 24, line 184: Is the matrix N_z related to the number of endmembers N_λ? If yes, could you state it explicitly in the text? If not, wouldn't be better to use a different letter?

Line 222: the term '*unconstrained*' should be substituted with '*bound-constrained*'.

Line 227: as stated above by the authors (line 220), the case $d_k = -g_k$ has not been explored in this study. Perhaps it is better to remarks this to the reader also in line 227 to avoid confusion. E.g., "... if the iteration increment k = 0 (not investigated here), or..".

Line 243: the term '*unconstrained*' should be substituted with '*bound-constrained*'.

Line 252: the equation number should in within brackets, e.g., equation (42).

Line 262: the compositions (NCKFMASHTO, KNCFMASTOCr, and FMATOCr) should be explained here, since they refer to the oxides components and it might not be intuitive: N = Na2O; C = CaO; etc. Moreover, there should be an explicit reference to Table 1.

Line 271: the term '*unconstrained*' should be substituted with '*bound-constrained*'.

Line 273: The acronyms 'SLSQP' and 'CCSAQ' should be explained before their first use.

Table 1: Temperature should be expressed in [K] not [°C] to be consistent with eq. 2. However, if the authors prefer to keep the units of measurements typically used in metamorphic petrology (kbar and °C) they should state it in the caption of Table 1.

Figure 2: It would be useful to report the dimensionality below the mineral e.g., clino-amphibole (dimensionality 10) or (10 oxides composition).

Line 281: the term '*unconstrained*' should be substituted with '*bound-constrained*'.

Figure 3: It would be useful to report the dimensionality also in this Figure.

Lines 292, 293, 300: the terms '*unconstrained*' should be substituted with '*bound-constrained*'.

Figure 4. How do you compute the local minimum of the solvus (yellow dots)? Have you obtained them with THERMOCALC using the Holland et al. (2018) database? The reference of these data points must be added.

Line 304: when referring to figures and tables you should be consistent throughout the manuscript: either Fig. or figure; Figure or figure; Table or table, etc...

Line 313: Figure 5A to 5C.

Line 315: 5A, 5B, 5C.

Line 316: 5D, 5E, 5F.

Figure 5: It would be useful to report the dimensionality also in this Figure.

Lines 319, 325, 328: the terms ‘*unconstrained*’ should be substituted with ‘*bound-constrained*’

Line 330: could you elaborate the ≥ 3 factor improvement? Why is it different from the one reported in the abstract?

Competing Interests: This statement should be more explicit e.g., ‘BK (co-author) is a member of the editorial board of GMD’.