Response to Reviewer Comments 2

We thank the reviewer for evaluating our manuscript and for the constructive comments. Note that we use the abbreviation **RC2** for reviewer comments and **AR** for our authors' response in the following. Removed text is shown in red, e.g., ~~this text has been removed.~~. New text is shown in blue, e.g., this text has been added.

RC2: I read with great interest the manuscript entitled "RHEA v1.0: Enabling fully coupled simulations with hydro-geomechanical heterogeneity" by Espejo and co-workers.

Despite I acknowledge the efforts from the authors, I am adivising for a major revision before the paper can be consider for its publication in GMD. The main criticism is that the paper lacks the scientific novelty required to make a major contribution to the related community. This is not a limitation of their approach (I think), but rather stems from the authors' choice of the examples discussed in the paper. Indeed, while claiming that their workflow contribute to advance the scientific computing efforts for complex subsurface applications, they limited their discussion to simplistic analytical examples. Terzaghi consolidation is a relatively simple benchmark, which should only be used to validate the physics implementation of their numerical tool. However, this is not the topic of the manuscript, given that the authors relied on existing modules (Porous Flow and Tensor Mechanics). Their realistic example is also a synthetic and simple one, 2 dimensional and with no clear tangible application.

I am saying this, cause the reader is left with the (wrong?) impression that the main contribution of the manuscript is the development of a python script binding MOOSE's objects, which to my opinion does not satisfy the minimum scientific level for a publication (it would rather fit as an internal report). This said, I would warmly advise the authors to re-organize the manuscript in a way to better convene the main message of their work, and, in doing so, to prove their generic sentencing as "... Our work is a valuable tool to assess challenging real world hydro-geomechanical systems that may include different levels of complexity like heterogeneous geology with several time and spatial scales and sharp gradients produced by contrasting subsurface properties. ...", for which I could not find any concept of proof in the text.

AR: We agree and therefore we appreciate the opportunity to clarify the novelty of our work.

1. While RHEA utilizes existing modules of the MOOSE framework (namely Porous Flow and Tensor Mechanics), we significantly changed the underlying MOOSE code (directly in C++) to integrate new material objects that, for the first time, unlock modelling of spatially distributed heterogeneity of mechanical in addition to hydraulic properties.

2. To ease pre-processing efforts arising from this improvement, we developed a Python-based, automated workflow which uses standard data format to generate input files that are compatible with the new material objects in MOOSE format. This helps users integrate spatially distributed properties into the modelling workflow.

3. We verified the correctness of our novel application with newly developed, analytical benchmark problems. This includes, for the first time, vertical heterogeneity and illustrated its performance using a sophisticated 2D example with distributed hydraulic and mechanical heterogeneites.

This novel development results in a numerical simulator that we call Real Heterogeneity App (RHEA). To the best of our knowledge, comparable open-source and verified simulators for coupled and fully distributed hydraulic and geomechanical heterogeneities have not been documented in the peer-reviewed scientific literature yet.
Nonetheless, the comment made by the reviewer showed us that the novelty of our work was insufficiently formulated in our manuscript. We therefore take the opportunity to improve our manuscript as follows.

Suggested revision at line 78: "However, it has not yet been extended and verified for the simulation of spatial heterogeneity of mechanical parameters. In other words, despite PorousFlow is able to handle spatially distributed heterogeneity of permeability and porosity, it does not support spatially distributed heterogeneity of mechanical properties such as bulk and Young's moduli."

Suggested revision at line 83: "RHEA is based on MOOSE's modular ecosystem and combines the capabilities of Porous Flow and Tensor Mechanics with material objects that are newly developed in our work and provide the novel ability to allocate spatially distributed properties at element-resolution in the mesh. To achieve that, we significantly changed the underlying MOOSE code of Porous Flow and Tensor Mechanics by integrating new C++ objects. To ease pre-processing efforts arising from this improvement, we developed a Python-based, automated workflow which uses standard data format to generate input files that are compatible with the material objects in MOOSE format. Finally, we verified the correctness of RHEA with a newly developed, analytical benchmark problems allowing vertical heterogeneity and illustrated its performance using a sophisticated 2D example with distributed hydraulic and mechanical heterogeneity."

RC2: (...) they limited their discussion to simplistic analytical examples. Terzaghi consolidation is a relatively simple benchmark, which should only be used to validate the physics implementation of their numerical tool.

AR: We agree that Terzaghi's problem is a simple benchmark problem, however it provides the opportunity to verify the hydro-geomechanical coupling of numerical solvers, see (Haagenson et al., 2020; Park et al., 2019; Ferronato et al., 2010; Kim et al., 2015; Blanco-Martín et al., 2017; Ma et al., 2017). In our contribution, we decided to verify the hydro-geomechanical coupling of RHEA which is based on combining Porous Flow and Tensor Mechanics as this numerical implementation has not yet been verified in the peer-reviewed scientific literature to the best of our knowledge.
Because we recognise the lack of complexity of Terzaghi's problem, we developed and illustrated two new benchmark examples that increase in complexity. The first uses analytical solutions to describe one-dimensional (vertical) heterogeneity, the second shows a two-dimensional system based on real-world data. We believe that these examples sufficiently verify RHEA and note that developing higher levels of complexity for benchmarking is out of scope for this manuscript (see for example (Green et al., 2021)).

Suggested revision at line 171: "The tests were designed to gradually build up complexity and cover the typical spectrum of consolidation problems. The first test, the classical Terzaghi's problem, is simply used as a basic benchmark of the hydro-mechanical coupling in RHEA. Later sections we illustrate the full possibilities of RHEA on spatially-heterogeneous systems in one and two dimensions.

RC2: (...) However, this is not the topic of the manuscript, given that the authors relied on existing modules (Porous Flow and Tensor Mechanics).

AR: While RHEA relies on existing physical modules of the MOOSE framework, we developed new materials that extend the capabilities to those physical modules. Further development of existing capabilities forms one of the fundamental and desired characteristics of the MOOSE framework, see previous MOOSE based numerical solvers that were built in a similar way (Keniley and Curreli, 2019; Slaughter and Johnson, 2017; Jacquey and Cacace, 2017).

Suggested revision at line 7 (Abstract): (...) "element-resolution hydro-geomechanical properties in coupled simulations. To achieve that we developed new materials that extend the capabilities of the current MOOSE physical modules."

Suggested revision at line 81: "The aim of this paper is therefore to develop, verify and illustrate a novel and generic workflow for modelling fully coupled hydro-geomechanical problems allowing the inclusion of hydraulic and geomechanical heterogeneity inherent to realistic geological systems. This was achieved by extending the current capabilities of the MOOSE of two its native physical modules, namely Porous Flow and Tensor Mechanics. We call this workflow RHEA" (...)

RC2: (...) Their realistic example is also a synthetic and simple one, 2 dimensional and with no clear tangible application.

AR: The Herten analog is a high resolution hydraulic dataset assembled from a real outcrop, as described in section 4.4.1. We decided to use this well-knwon aquifer analog due to the fact that we could not find any other suitable datasets that integrate full hydro-geomechanical heterogeneity. While we agree that this example is synthetic, the aim was to (1) illustrate how to generate the data files to simulate with RHEA from real data sets, (2) demonstrate increased spatial complexity and sharp gradients. The example could be extended to three dimensions, but it was reduced to two dimensions as this is sufficient to demonstrate RHEA's capabilities and facilitates visualisation of the results.

The aim of this manuscript is to document the development and verification of a simulator for fully distributed heterogeneity, so we believe further modelling of a real problem is beyond the scope of this contribution. We intend to do this in a follow-up study.
Regarding a tangible application, we are currently utilizing RHEA to model land subsidence due to heavy groundwater extraction. We calibrate our models by fitting hydro geomechanical parameters generated by RHEA's workflow to vertical displacement data sets which have fine spatial discretization. RHEA's workflow dramatically simplifies the model fitting since we are able to allocate material properties to each displacement measuring point and the area around it.

Suggested revision at line 272: "The last example aims to study and illustrate the performance of RHEA's with a real data set.~~The 2D consolidation problem was solved with RHEA, integrating the multi-facies realizations and material properties of the Herten analog (Bayer et al., 2015)~~ This example illustrates how to generate input files with the developed workflow and demonstrates the potential of RHEA in increased spatial complexity and sharp gradients. While the Herten analog is a 3D data set, the example was reduced to two dimensions to facilitate visualization. Regardless, simulations in three dimensions would not modify the presented workflow. Hence, the 2D consolidation problem was solved with RHEA, integrating the multi-facies realizations and material properties of the Herten analog (Bayer et al., 2015). Although the data set does not contain geomechanical subsurface properties, the hydraulic conductivity varies in six orders of magnitude which represents a sufficient proof of concept for RHEA.

Suggested revision at line 341: "With RHEA a number of future potential applications rise, for instance, land subsidence is a process that can occur due to progressive consolidation due to slow downward percolation over several soil layers due to anthropogenic decrease of the system pressure. The process highly depends on the spatial distribution of the geomechanical properties of the subsurface, RHEA's workflow can potentially simplify such numerical simulations."

Suggested revision at line 345: " However, RHEA could potentially be extended to include also thermal processes and three dimensional simulations."

RC2: This said, I would warmly advise the authors to re-organize the manuscript in a way to better convene the main message of their work, and, in doing so, to prove their generic sentencing as "... Our work is a valuable tool to assess challenging real world hydro-geomechanical systems that may include different levels of complexity like heterogeneous geology with several time and spatial scales and sharp gradients produced by contrasting subsurface properties. ...", for which I could not find any concept of proof in the text.

AR: The aim of this contribution is to document the development of RHEA and illustrate how realistic geology leading to full and distributed hydro-geomechanical heterogeneity can be modelled. Starting from a relatively simple example (Terzaghi's problem), the level of complexity was increased until a real-world example was presented. We note that sharp gradients can be seen in section 4.2 where hydraulic conductivity varies over four orders of magnitude and are further illustrated in section 4.4 where the hydraulic conductivity varies across six orders of magnitude.

To better reflect this aim, we have revised the statement in line 12 as follows: Our work is a valuable tool to assess challenging real world hydro-geomechanical systems that may include different levels of complexity like heterogeneous geology with ~~several time and spatial scales and~~ sharp gradients induced by contrasting subsurface properties.

Suggested revision at line 170: "The tests were designed to gradually build up complexity and cover the typical spectrum of consolidation problems. In two of this examples RHEA's performance on simulations with sharp gradients is tested. First, a one dimensional consolidation problem where the hydraulic conductivity varies in four orders of magnitude between layers and a second two dimensional example with realistic heterogeneity in which the hydraulic conductivity of the facies varies in six orders of magnitude."

In terms of organisation, we have attempted to structure our manuscript in a logical way from development to verification with increasing complexity abd therefore we have not changed the organization.

RC2: * Abstract - sentence at lines 4-5 - it requires some reworking. Stating that there are no simulations considering heterogeneity in the subsurface is simply not true (an extensive literature research is required here). In addition, it is not clear what they mean by "verification".

AR: We agree. For further reference we quote our sentence in line 4-5: "However, implementation and verification of full heterogeneity of subsurface properties using high resolution field data in coupled simulations has not been done before."

We agree that this sentence may not be clear enough. Specifically, the "full" heterogeneity refers to coupled hydraulic AND mechanical heterogeneity, for which there are no open source numerical simulators reported on in the peer-reviewed scientific literature. A close example would be other MOOSE based simulators, where the user can potentially define spatial distributed mechanical parameters by specifying different materials when the mesh is generated (either with MOOSE or other mesh generator software), this workflow works well for simplified systems, for instance layered geology. The latter is illustrated in GOLEM Jacquey and Cacace (2017) which is also a MOOSE-based derivative. However, if realistic geology with complex and naturally shaped geometries is introduced, defining materials when the mesh is generated becomes a significant effort. This is why we introduce our Python workflow in which the user defines location of the properties by specifying Cartesian coordinates as well as the values. The generated files are MOOSE compatible, imported into the simulation and automatically assigned to the appropriate mesh by the dedicated material objects included in RHEA.
Similar workflows have been used in the past, but are limited to coupled hydraulic simulations (only for hydraulic conductivity and porosity, see (Maier et al., 2005; Höyng et al., 2015)). To the best of our knowledge, RHEA provides this capability for coupled hydraulic and geomechanical properties.
We also agree that "verification" may not be an intuitive term to use in this context. Further explanation is added.

Line 32: "However, integrating spatial material properties to numerical tools typically is an arduous task since natural shaped geological formations are made of complex geometries produced by natural processes around them. Advance proprietary numerical tools with a graphical interface such as COMSOL Multiphysics (1998), can format material data to the simulation by importing text files to the software. However in this case, an automatic interpolation between neighbor materials is internally performed, which may lead to unwanted results. To the best of the authors' knowledge there is no open source numerical tool able to integrate full heterogeneity of complex geologic formations for all hydro-geomechanical parameters."

Line 85: "We then compare RHEA's simulation results (verify) ~~verify RHEA~~ with one and two dimensional analytical solutions, and propose a benchmark semi-analytical solution to investigate RHEA's performance when sharp gradients are present."

RC2: * Introduction - sentence at lines 26-27 - also this sentence is not true ("infeasible").

AR: We agree and will revise accordingly:

Line 26: (...) "so that fine spatial discretization around fractures is needed in certain numerical models, resulting in ~~infeasible~~ expensive computational demands"

RC2: *Introduction - sentence at lines 65-67 - The coupling among physics is not done automatically but via off-diagonal components in the system's Jacobian matrix.

AR: We agree and corrected our text accordingly:

Line 65: (...) "each physical process (or its partial differential equation, PDE) is treated separately as an individual MOOSE object and coupling is performed ~~automatically~~ by the back end routines of MOOSE."

RC2: * Paragraph 3 - sentence at line 136 -Material properties are defined at the element level by default in any FEM application.

AR: We agree and revised as follows:

Line 136: (...) ~~We accomplished this by introducing material properties that can allocate data at each mesh element.~~
(...) "We accomplished this through new MOOSE-based materials functions able to allocate data in each element of the mesh based on a pre-generated input file. "

RC2: * Paragraph 3 - sentence at line 155 - Why the size of the mesh needs to match the coverage of the sampling data? Is that a limitation of a naive implementation of the interpolation routine used within the workflow?

AR: Since the materials properties have to be assigned at every element, elements with unassigned material properties would raise an error. RHEA automatically linearly interpolates the value of the material property to the unassigned element. Hence, the user has to be careful that the dataset matches the mesh discretization size. Otherwise, interpolated values will be assigned which could lead to significant errors. If further refinement of the mesh is necessary, the mesh adaptivity of MOOSE can be activated, as described in section 4. Hence, we extended our previous statement as follows:
We plan to amend this statement as follows:

Line 156: RHEA may assign unwanted property values, ~~since it uses a linear interpolation between neighbouring values.~~
"since RHEA will automatically linearly interpolate the values provided to the mesh. Thus, if the initial mesh discretization does not match the user-supplied samples, interpolated values are assigned, which could lead to unexpected behavior."

RC2: Why rephrasing equation 8 in terms of the hydraulic conductivity? It does not match the formalism used in the previous paragraph ...

AR: We agree and will revise accordingly:

Line 106: We express equation 3 in terms of hydraulic conductivity.

$$\boldsymbol{q}_d = \phi(\boldsymbol{v}_f - \boldsymbol{v}_s) = -\frac{\boldsymbol{k}}{\mu_f \rho_f \boldsymbol{g}}(\nabla p_f - \rho_f \boldsymbol{g}) \,, \tag{3}$$

Line 107: "where $\mathbf{v}_f$ and $\mathbf{v}_s$ are the fluid and solid matrix velocities respectively; ~~**k** is the permeability tensor; μ_f is the dynamic viscosity of the fluid;~~ **k** is the hydraulic conductivity tensor; "

We appreciate the time and effort made by the reviewer and therefore acknowledge him in our acknowledgement.

References

L. Blanco-Martín, J. Rutqvist, and J. T. Birkholzer. Extension of tough-flac to the finite strain framework. *Computers & Geosciences*, 108:64–71, 2017.

M. Ferronato, N. Castelletto, and G. Gambolati. A fully coupled 3-d mixed finite element model of biot consolidation. *Journal of Computational Physics*, 229(12):4813–4830, 2010.

C. P. Green, A. Wilkins, J. Ennis-King, and T. LaForce. Geomechanical response due to nonisothermal fluid injection into a reservoir[U+2606]. *Advances in Water Resources*, 153:103942, 2021.

R. Haagenson, H. Rajaram, and J. Allen. A generalized poroelastic model using fenics with insights into the noordbergum effect. *Computers & Geosciences*, 135:104399, 2020.

D. Höyng, H. Prommer, P. Blum, P. Grathwohl, and F. M. D'Affonseca. Evolution of carbon isotope signatures during reactive transport of hydrocarbons in heterogeneous aquifers. *Journal of contaminant hydrology*, 174:10–27, 2015.

A. Jacquey and M. Cacace. Modelling fully-coupled thermo-hydro-mechanical (thm) processes in fractured reservoirs using golem: a massively parallel open-source simulator. In *EGU General Assembly Conference Abstracts*, page 15721, 2017.

S. Keniley and D. Curreli. Crane: A moose-based open source tool for plasma chemistry applications. *arXiv preprint arXiv:1905.10004*, 2019.

J. Kim, E. Sonnenthal, and J. Rutqvist. A sequential implicit algorithm of chemo-thermo-poro-mechanics for fractured geothermal reservoirs. *Computers & geosciences*, 76:59–71, 2015.

T. Ma, J. Rutqvist, C. M. Oldenburg, W. Liu, and J. Chen. Fully coupled two-phase flow and poromechanics modeling of coalbed methane recovery: Impact of geomechanics on production rate. *Journal of Natural Gas Science and Engineering*, 45:474–486, 2017.

U. Maier, A. Becht, B. Kostic, C. Burger, P. Bayer, G. Teutsch, and P. Dietrich. Characterization of quaternary gravel aquifers and their implementation in hydrogeological models. *IAHS PUBLICATION*, 297:159, 2005.

C. Multiphysics. Introduction to comsol multiphysics®. *COMSOL Multiphysics, Burlington, MA, accessed Feb*, 9:2018, 1998.

C.-H. Park, T. Kim, E.-S. Park, Y.-B. Jung, and E.-S. Bang. Development and verification of ogsflac simulator for hydromechanical coupled analysis: Single-phase fluid flow analysis. *Tunnel and Underground Space*, 29(6):468–479, 2019.

A. Slaughter and M. Johnson. Pika: A snow science simulation tool built using the open-source framework moose. In *AGU Fall Meeting Abstracts*, volume 2017, pages C22B–08, 2017.