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Reply to the reviewer's comments:

We would like to thank Angelo De Santis and the anonymous reviewer for the additional careful review of this paper. We appreciate that the review by Angelo De Santis allows us to make the new approach available to a much broader audience and we are again, extremely grateful for the patience and detailed feedback providing useful criticism and suggestion for modifications.

We are also very grateful for the anonymous second review in particular for highlighting potential misunderstanding stemming from the original title of the article and the need for explicitly mentioning the difference between Hu et al 2020 and the generalised multiscale approach. We feel that the additional explanations are important and were indeed lacking in the earlier version.

Please find below the address of the specific points raised by the reviewers.

Yours kindly Klaus Regenauer-Lieb

Annotated NOTES for "Cross-Diffusion Waves as a trigger for Multiscale, Multi-Physics Instabilities: Theory" *by* Klaus Regenauer-Lieb et al.

Angelo De Santis (Referee)

Line 1: We propose a non-local, meso-scale approach for coupling multiphysics processes across the scales. I find this sentence a little contradictory: "non-local meso-scale approach"... that deals with "...processes across the scales." I think a more clear statement is needed, especially because it is the first!

Reply: *Thanks for pointing this potential confusion out: The term "non-local" only speaks to a special applied mathematics or mechanics and physics of solids community and "meso-scale" has different meanings in different communities and is thus confusing. The sentence is now simplified to "*We propose a multi-scale approach for coupling multiphysics processes across the scales."

The term nonlocal reaction-diffusion equations is also now defined much later in the text (line 353 ff in the revision with highlights of changes) and a reference has been added.

Line 54: strange that the "early work" is referred by a more recent paper (Tse and Rice 1986) than Dieterich

Reply: *The qualifier "early" is removed*

Line 59: What do you mean for "geophysical solids"? I could understand it, but as a geophysicist it is unusual. Do you simply mean "earth science" or "solid earth" or what? I do not say that this term is wrong but it is not commonly used in geophysycs.

Reply: *Changed to solid earth community*

Line 65 following: How far is your theory from the accepted continuum mechanics? Which are the differences and similarities? At first glance, the main differences are: a) one concerns with continuous processes, while the other concerns with discontinuous, intermittent, puntual processes; and b) you add also thermal and chemical aspects. But nothing explicit and clear is said. I think one-two sentences, at least in the Conclusions, would be of great help for any potential reader.

Reply: *The classical theory of standing waves accepted in continuum mechanics is a special case of the present approach which comes out for a relatively narrow parameter space. This indicates perhaps that processes in nature have a much richer solution space than anticipated by the classical theory of localisation. This shortcoming of the classical theory (overlooking two different forms of instabilities) is not addressed in the current paper as it requires additional derivations.*

The current manuscript only addresses the two main problem in the classical approach. The first is that the classical theory disregards propagating waves in the solution space, the second is that the solution is mathematically ill-posed due to the infinite response of strain-rate in shear, or overpressure in compression, and the third that is axiomatic and not based on physics processes as is preferred in geosciences because of the need for extrapolation on longer time scales inaccessible to the observer.

The standard approach in the solid mechanics community is to either add an empirical material length scale (e.g. related to strain gradients) or use numerical diffusion to capture the singularities. Only few researchers have attempted to regularise the approach by referring to physics phenomena through introduction of a self-diffusion process or a chemical reaction term or both. This is a hot topic and now better explained through an additional paragraph on line 56 in the marked up revision. We also come back to the point on line 353 ff.

Line 71: here you say that you investigate the meso-scale ... from the... solution of the macro-scale. In short, you affirm that the study of a scale has effect in understanding the features of another scale. This is not obvious and should be better explained and clarified

Reply: *This has now been amended and additional text added*

Line 71: his sentence is not clear:
"the scale .... is defined by ...[their] own ... scales". Would do you mean:
"we propose that each of the THMC processes is defined by [its] own characteristic diffusion time/length scales"?
In addition, I have clear idea about diffusion time (in terms of the solution of diffusion equation), but how do you define the length scales? This also is not clear.

Reply: *Changed to "*In order to define the separation between the meso- and macro-scale of a THMC coupled problem, we propose that the scale for each of the THMC-processes is defined by its own characteristic diffusion time/length scales \citep{JCSMD1}. The THMC diffusion length scale is thereby related to the time scale of a considered THMC process as defined by the proportionality to the square root of the diffusivity multiplied by the process time."

Figure 3 caption: In the main text you speak about extended length scales: here the length scale is rather short. How do you combine the two points?
In addition: I notice with respect to a majority of lines there are also some hortogonal (and other inclined) lines, which are not reminiscent of a standing wave or are difficult to be explained.

Reply: *This is well spotted. Results of our detailed field work are now available and cited in the caption. The standing waves are the exception rather than the rule both from the linear stability analysis performed by us (to be discussed in a forthcoming contribution) and as well from geological observations, where irregularly spaced deformation bands are more frequently encountered. The standing waves are normally found far away from the faults and form the smallest spacing (around 10 cm) in our field example. The figure has been replaced and more explanation is added to the caption including reference to the new publication and the question of scale is now clarified in the caption.*

Line 326: **i**t is not clear. Do you mean "... H_THMC corresponding to the conditions of Table 1"? Or what?

Reply: *In order to generalize the approach, we propose that all reaction-diffusion equations in Table 1 are strongly coupled. We construct a composite multi-scale THMC diffusion wave operator ^HTHMC from the four reaction-diffusion equations in Table 1.*

$$\hat{H}_{THMC} = -\zeta_i \sum_{i=1}^{N} \nabla^2,$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ and i refers to the individual thermodynamic THMC process.

The wave operator is now also discussed in further details on line 353 following.

Line 393: here t is generic. How do you define numerically the length scales? Do you replace it by the diffusione time? Or what?

Reply: *The time t is now defined on line 430 ff in the revised annotated manuscript*

Line 399: I do not understand: you are comparing "cross-diffusion length/time scales" with "self-diffusion length scales". The former includes space and time scales, the latter only space scales.

Reply: *It is now consistent*

Line 501: This sentence comes out of the blue. You should refer to the second part, where, I presume (I did not yet read it), you provide more convincing arguments. I would also suggest some more clarifying sentence concerning this point.

Reply: *The sentence is now clarified:* see line 553 in the annotated revisions.

In addition all minor typographical errors have been corrected.

Response to Anonymous(Referee) comments

Suggestions for revision or reasons for rejection (will be published if the paper is accepted for final publication)

This constitutes my review of the Regenauer-Lieb et al manuscript “Cross Diffusion Waves …: Theory. This is paper 1 of a two-paper series. I enjoyed reading this paper and feel that it should be accepted with minor revisions. I detail some minor corrections below (these are minor). The paper is a good companion to the Solid Earth Special Issue deriving from the recent GEOPROC conference in Ultrecht.

Two aspects present themselves which the authors should concern themselves in the revisions. First, much of the theory and discussion in this paper mirrors the treatment in the recent Hu et al. paper (J. Mechanics Phys Solids 135, 2020). The authors should discuss how the present paper differs in content from the Hu et al. paper.

Reply: *The revised version now explains the present work in relation to the Hu et al.(2020) paper. Differences in the present work are closing the link (and spelling out the differences) to the classical established theory of Hill et al. and following authors (new paragraph following line 56 in the marked-up revised manuscript as well as the paragraph following line 353), establishing the case for the generalized multiscale THMC problem and linking up with other cross-diffusion formulations from different disciplines. The intellectual contribution of the derivation of the cross-diffusion term from two-scale mixture theory in Hu et al.(2020) is now also more explicit. A paragraph has been added to clarify the rationale to repeat the mixture theory approach in generalised form here (line 365 in marked up revision). This approach constitutes an important difference to other attempts (including our own) at closing the ill-posed reaction-diffusion problem through ad-hoc assumptions.*

Second, I feel that the “cross-diffusion” aspect of the wave propagation is confusing and potentially ill-suited to describe the onset of THMC instabilities. The authors accurately describe the “cross diffusion” matrix in analogy with the cross diffusion (non diagonal) terms arising in chemical diffusion as occurs in concentrated brines or melts e.g. These represent “linear” couplings between fluxes and forces in the Onsager sense. As such the terms in the matrix do not describe the (by necessity, as described by Prigogine) non-linear couplings that arise from 1. Non equilibrium conditions and 2. The existence of coupling feedbacks. I think its important to distinguish excitability (nonlinear growth of perturbations) which would be described by the reaction rate terms in their Table 1 or in their equations (21). I think this is well discussed in the Tsyganiov reference the authors include. Thus I question the linkage of “cross diffusion” with instability given in the title.
The same would be true of the “acoustic tensor “ plasticity approach of Hill and Rudnicki and Rice – they discuss the “uniqueness” of plastic instabilities but a priori assume the “existence”.

The phenomena discussed in this paper are related to the compaction/density waves discussed by Dan McKenzie in 1984 and in that case, the instabilities require a nonlinear coupling of porosity with permeability – surely the linear requirement of the cross diffusional matrix (which is explained better in the HU et al paper) preclude this type of instability? The authors may wish to elucidate these concerns, and hopefully these don’t muddy the waters but lead to a clarification. Certainly the non diagonal terms in the THMC matrix in the authors Table 1 are important considerations in the propagation of soliton-like waves, but by themselves they don’t describe the onset of instability leading to the development of such waves???

Or am I missing something?

Reply: *We would like to thank the reviewer very much for highlighting this important potential misunderstanding of the paper (and the title) which we did not foresee. The aspect of the necessity of non-linear reaction terms is indeed fully acknowledged. It is the subject of the companion article providing a step-by-step introduction into the theory of excitable waves stemming from the THMC reaction terms and putting proper reference to the FKPP work and the subsequent work in the Russian literature. This discussion was beyond scope for the first part. The important reference to excitation waves as discussed in the companion paper is now highlighted on line 11, 40 and 353 ff in the revised manuscript.*

The title was meant to convey the important fact that without cross-diffusion terms no new type of soliton-like (quasi-soliton or cross-diffusion) wave is generated (triggered) given the existence of excitable waves. We appreciate, however, that this point only becomes clear after reading the paper and one could misunderstand the title. We therefore changed the title, added a sentence at the end of the abstract and further explanation to the wave operator discussion on line 353 in *the annotated revised manuscript. The wave operator was originally introduced to highlight the role of the non-diagonal terms which were overlooked in our early work on compaction bands.*

This early work on the standing wave solution of the Korteweg-de Vries (KdV) equation as an explanation for compaction bands in nature considered indeed an extension to McKenzie's theory by using a nonlinear rheology (we obtained analytical solutions with power law exponent 3 reaction term). It resulted in unphysical infinite overpressure spikes on the instabilities. On line 48 following we now highlight this problem of both our early work on the KdV equation and the axiomatic classical localisation theory of plasticity theory by Hill and Rudnicki and Rice. In the new paragraph following line 55 we also discuss the limits of our own earlier work to improve this approach and come back to the important point on line 353.

Because of the proposed importance to understand localisation bands in nature our team and our collaborators have since tried to regularise the problem for the purpose of obtaining numerically stable solutions. Generalised equations were analytically not tractable and numerical work was therefore crucial. Several solutions that worked for some cases were found. The intention of Hu et al.(2020) and the present work is to close this ill-posed problem by considering the nonlocal nature of the reaction term.

In Hu et al. (2020) we presented pioneering work for HM coupling. The current work is proposing a closure for all considered THMC extensions through generalisation of cross-diffusion terms proposed in Hu et al.(2020). The work also spells out clearly the differences to earlier work in localisation theory based on acceleration waves missing in Hu et al (2020). Finally, this work also attempts to provide the reader a bridge to the rich published literature on quasi-solitons where many more aspects of cross-diffusion waves are discussed in different communities, which should be easily digestible given our introduction. This intention is now highlighted more specifically in various sections of the revised version to elucidate the important differences, hopefully without distracting from the key ideas presented in this work.

This article is indeed all about the non-diagonal terms in the THMC matrix and the consideration of the propagation of soliton-like waves which was not yet clearly addressed before. The interesting aspect is that without off-diagonal terms but with non-linear source terms no cross-diffusion waves are triggered but only solitary waves with Hopf and Turing bifurcations. New work by our team has provided proof of this statement for the generalised case of poro-mechanics applications. Only by inclusion of cross-diffusion (acknowledging higher order reactive source terms for the solid skeleton and a linear fluid reaction term) excitable waves with quasi-solitonic behaviour are triggered. As our new work is only in draft manuscript form we refer in the revision on line 363 to Tsyganov (2007) who identified the important finding first for the mathematically similar Fitz-Hugh Naguno system.

The companion paper is more of a step-by-step introduction as it starts indeed with a summary of the theory of excitable waves and then goes over into a discussion of the influence of the non-diagonal terms in the diffusion matrix.

Line 42 – the authors may wish to consider a consistent way of referring to the second, companion paper (e.g., Paper 1, and Paper 2)

Reply: *The second paper is now named "companion article" throughout the text.*

Line 79 – omit the second "s" in "systemss"

Reply: *Done*

Line 89 – sentence is confusing ("processes travels"??)

Reply: *it now reads that the information disperses*

Line 95 – omit "s" in details; omit comma after diffusion

Reply: *Done*

Line 109 – omit semi colon and instead use parenthesis to be consistent with earlier terms in the sentence, i.e., "chemical driving forces (chemo-taxis)"

Reply: *Done*

Line 110 – omit “Thermal, Hydrodynamic, Mechanical, and Chemical” as abbreviation has been defined previously

Reply: *Done*

Line 123 – omit comma after “physics”

Reply: *Done*

Line 134 – put references in parentheses.

Reply: *Done*

Line 253 – It is confusing as to what is meant by “former” and “latter” with respect to the previous sentence; please rewrite

Reply: *Done*

Line 276 – the creeping flow assumption ignores the acceleration terms in the Navier-Stokes equation, but there still can be effects of “gravitational acceleration”, i.e. creeping flow in a gravity field.

Reply: *Done*

Line 285 – The phrasing “The compatibility condition relating jumps…” is not a complete sentence

Reply: *Done*

Line 293 – I believe you want to make the phrase “It follows from Eq. 7” the start of a new sentence

Reply: *Done*

Line 324 – “tabulated in Table 1. The reaction rates…”?

Reply: *Done*

Line 326 – there is no operator H-hat-sub”THMC” in Table 1.

Reply: *The intention of the introduction of the wave operator, based on the self- diffusivities defined in Table 1, was to build up for the following discussion on the necessity for considering cross-diffusion coefficients from the nonlocal reactive source term. This operator maps the excitation waves into a new space that when including cross-diffusion coefficients generates quasi-solitons. The operator was originally introduced as a mathematically more succinct form of the lengthy step-by-step “convolution wave filter” discussion in the companion article. This information was obviously missing and is now given on line 353ff .*