Response to "A Comment on Meeting the Contact-(Mechanics) Challenge"

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In his comment [1] on the Contact-Mechanics Challenge [2], Ciavarella reports his difficulties to reproduce one data set of the submission of one contributor, namely the gap-load relation by Persson. The comment could convey the impression that Persson's model was not fully defined, which might imply by a worst-case extension that Persson's data was fudged. After all, the term *fudge factor* appears three times in the comment. I respond to the comment as the corresponding author of the study, who designed the challenge, who collected all data from all contributors, who prepared all figures, and who ultimately wrote the paper with helpful feedback from many co-authors and steady encouragement from two Tribology Letters editors.

First and foremost, I feel the desire to state that my own reference data had not been disclosed to anybody before I collected the results. In some cases, I noticed potential errors in the submissions, which appeared unrelated to the used methodologies themselves, but seemed to be unit-conversion problems or similar misunderstandings. In these cases, I told the contributors where I believed the errors to be, asked them to consider my findings and to resubmit. This was done without the passing on of any reference data or of hints if some predicted number was too large or too small.

Persson was the second participant of the challenge to submit his data. There was no need to ask for resubmission, because his data matched my full Green's function molecular dynamics (GFMD) [3] based simulations within the small deviations that usually occur when both theory and simulations are carefully conducted. I

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can thus assure that there was no fudging in Persson's or any other submission. As a personal note I may add that I used to be skeptical of the good match of his theory with experimental data myself. This is why I asked Persson in 2011 to make predictions on the Reynolds flow through the thin gap between a randomly rough surface (defined with mathematical precision) and an elastic manifold with equally well-defined elastic properties. During the write-up of this personal challenge, I did not share my data with him either, until I prepared the figures of the final write-up, which was published in Physical Review Letters [4]. This procedure between Persson and me is now established whenever we collaborate.

In his comment, Ciavarella asks for the *results to be completely accessible*. As the corresponding author of the Contact-Mechanics Challenge, I rewrote all model descriptions such that anybody with access to the internet and my modest background in contact mechanics would be in a position to reproduce the gist of every contribution. In some cases, it took many iterations and perhaps some frustration on behalf of my co-authors until I felt to be in a position to (roughly) reproduce each submitted data set from scratch. The one contribution that I would not dare trying to reproduce is the stunning experimental work of Greg Sawyer's group. As a two-left-handed theorist, I should not be allowed to enter a real laboratory.

However, it should be clear to anyone that a paper such as that summarizing the Contact-Mechanics Challenge needs to remain within a reasonable page limit and that this cannot be achieved if every theoretical approach is described in such excruciating detail that every reported number can be reproduced to several decimal digits. While it might have been appropriate to state explicitly that the elastic energy expression from

Reference [5] was taken, the description of Persson theory in the Contact-Mechanics Challenge closes with a clear reference to my own work with Wang [6], where we explain and extend Persson's submission, for anyone interested in more details.

Persson's submission happens to be the only one that I recomputed (with my own, independently written code), i.e., the one that Ciavarella reports to be irreproducible. I was dissatisfied by the small number of data sets that Persson had submitted and wanted to find out for myself how well his theory works for some of the properties that he had not predicted, since my own previous tests of Persson theory had not included adhesion. I, personally, had no trouble reproducing Persson's data.

Interestingly, Ciavarella ignored adhesion and yet compared his data to calculations that included it. While the Contact-Mechanics Challenge was addressed to scientists with the ability to model adhesion – other interfacial properties are indeed much more affected by moderate adhesion than the gap-load relation – I extend the Contact-Mechanics Challenge in this response to the gap-load relation without adhesion in order to properly address the comment. Results, which deviate quite strongly from those reported by Ciavarella, are presented in Fig. 1. GFMD and Persson theory only differ noticeably in the investigated pressure range when corrections are switched off completely. This, however, is well known and the reason why Persson introduced a correction to his theory – based on comparisons to experimental data (!) – to begin with [5]. This correction factor will be touched upon again later. Here, it shall suffice to state that slightly different versions of the correction factor produce results within the line width of the Yang-Persson data set shown in Fig. 1 and that different versions of Persson theory do *not* deviate by 500% as Ciavarella claims it to be the case. The original Persson prediction to the Challenge (blue line) touches the GFMD data (full circles) as well as the new, independent calculation conducted for this comment (long, dashed line) at the reference pressure of $p = 0.01 E^* \bar{g}$ and at larger pressures.

It is certainly not infrequent that an attempt to reproduce data from others first fails. If these data were produced by one scientist and then reproduced independently by another (who just successfully compared his own simulations to those of the rest of the world), one would assume it to be good scientific practice to troubleshoot the code that gave contradictory results. Ciavarella chose to write a comment instead.

It is not my job as organizer of the Contact-Mechanics Challenge to troubleshoot code of people, who do not succeed in reproducing the calculations of one of the
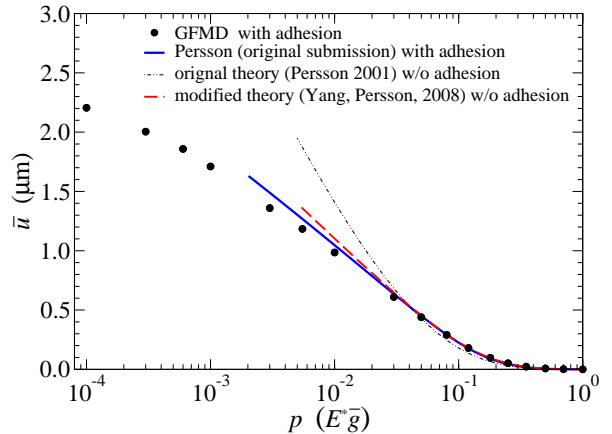

Fig. 1 Mean gap as a function of pressure as reported in Fig. 12 of the Contact-Mechanics Challenge [2] for the GFMD reference data and Persson's submission. Two new data sets are included, for which adhesion was not included.

participants. This is why, I cannot say why Ciavarella's attempt to reproduce Persson's gap-load relation failed. When ignoring adhesion, Persson theory is mathematically isomorphic to a diffusion equation with an absorbing boundary and thereby constitutes one of the simplest, standard partial-differential equation to be solved. It should not require much prudence to code it up correctly. However, the comment contains so many deficiancies that I consider it quite plausible that Persson theory was coded incorrectly as well. The first item that could be pointed out is that insufficient care was taken to reproduce correctly the title of the paper that was commented on. Unfortunately, there are many other mistakes and false or misleading statements that need correction. Since some of his views are widespread in the field, I seize the opportunity to address them in detail.

Linearity between relative contact area and pressure. In his opening paragraph, Ciavarella claims that the Greenwood-Williamson (GW) model explains linearity between the relative contact area $a_{\rm r}$ and pressure p in an elastic contact between nominally flat surfaces. It does so at best up to extremely small relative contact areas of $O(10^{-4})$ [7], while careful simulations of well-defined Gaussian surfaces (thus reflecting the conditions for which GW was constructed) reveal linearity up to $O(10\%)$ according to the relation $a_{\rm r} = \kappa p/E^* \bar{g}$. Here, κ is a unitless prefactor, which turns out close to two, E^* is the contact modulus, and $\bar{g}$ is the root-mean-square gradient of the surface [8,9]. For $a_{\rm r}$ exceeding 10%, corrections of order $O\{(p/E^* \bar{g})^3\}$

become noticeable [8,9] – in full accordance with Persson theory.

In contrast, the prefactor relating a_r and p in the GW model disappears with the root of the standard deviation of the peak heights σ_h [10] (I thank Ciavarella for pointing out the reference to me). This is why κ becomes arbitrarily small in the limit of macroscopic surfaces. However, there is a well-defined limit for the proportionality coefficient when σ_h tends to infinity, as can be concluded, for example, from Fig. 2 in Ref. [9]. Thus, while GW might result in a linear $a_c(p)$ relation, the prefactor is not meaningful, and, as such, no serious scientific paper or comment should claim the GW model to explain linearity between contact area and load in elastic contacts – even if modification of the GW theory [11,12] – which are qualitative in nature rather than corrective factors of order unity – are consistent with a linear $a_c(p/E^*\bar{g})$ relation at small p. I would always thank Greenwood for important contributions to contact mechanics. However, I do not see that GW has any predictive ability, even if the GW paper has guided our intuition for more than five decades and rightfully deserves credit for having opened up a new field of study.

False use and false interpretation of Persson theory. Ciavarella claims that *a normal reader gets the impression when reading Persson, that (that) equation* (no number given, but Ciavarella meant to refer to his equation 1, which relates pressure and mean gap) *should indeed hold for pure power-law spectra without roll-off.* I am not sure what a normal reader is and I somehow doubt that a good tribologist can be or even should be normal. However, an intelligent reader would only use the equation under those circumstances for which it was derived, i.e., when there are many decades of wave vectors on which the surface-height spectrum exhibits power-law scaling and also restrict its applicability to the appropriate pressure range. The used ratio of $q_s/q_r = 200$ ($q_{s,r}$ being the wave numbers associated with the short-wavelength cutoff and the roll-off, respectively) could simply not be enough for the equation to be very accurate. More importantly, the honest scientist, who had carefully studied Yang and Persson (2008) [13], would not claim that a normal reader could believe Persson's asymptotic $p(u)$ equation to be generally applicable. Yang and Persson explicitly write in their paper [13]: *For this reason it is important to accurately describe how U_{el} depends on $P_p(q)$ for all p, even if one is only interested in the relation between $\bar{u}$ and p for very small p.* Not only intelligent but also normal readers would use the $p(u)$ relation with caution and abstain from writing a comment that it produces inaccurate numbers.

A normal, fair-minded reader might not write either that *...require a number of "corrective or fudge factors", as Wang & Müser [3] themselves discuss at some length*, when the word *fudge* was not used in the cited paper and the authors clearly emphasized that a single corrective term remained of order unity.

Approximate nature of Persson theory. In his comment, Ciavarella writes: *Persson's theories remain always approximative.* It is not clear to me whether he meant to convey that *Persson's theory cannot be corrected such that it becomes an exact theory*, or, that *Persson claims his theory to be correct, but I am telling you that it is not.* Neither claim would be correct. I demonstrated a decade ago that Persson's approach reflects the leading-order terms of a rigorous perturbation theory (in form of a cumulant expansion) for linearly elastic systems [14]. The approach implicitly contains a recipe for how to correct the theory for the case where there is correlation. Since this recipe implies the coupling of the displacements at different wave vectors, it may not be practicable. The work did however reveal that Persson theory can be corrected systematically and thereby turned into an exact theory. In addition, I am not aware of a publication where Persson claims his theory to be exact – unless for full contact, which had been solved before.

In this context, but also because Ciavarella so heavily criticizes at various instances the use of fudge factors (in fact, Persson usually only uses one coefficient, which has remained pretty constant over time, while a true fudge factors would get adjusted for each new prediction), I wish to remind the reader that Persson theory is a renormalization group approach. Kenneth Wilson was awarded the Nobel prize in physics for his work on critical phenomena using the renormalization group (RG) in 1982. It is probably fair to say that Wilson's RG work, together with that of Fisher and Kadanoff, is the most influential work in statistical physics of the post Boltzmann-Einstein-Langevin area. In many RG approaches, including those pursued by Widom, Fisher, and Kadanoff, the main goal is to identify correct functional forms and correct exponents. A precise determination of prefactors is often not possible. Yet, Persson's approach can be turned into a quantitative theory with the help of a single coefficient of order unity. I, personally, find it quite amazing that such a minor fine tuning turns a rather simple RG theory into something that carefully working scientists can now use as a quantitative tool for the study of a rather complex problem. In retrospect, it is surprising that it took so long until the usefulness of RG was successfully applied to tribology and it is revealing how much difficulty many in the community have to apply it correctly.

Use of the random-phase approximation. In the opening paragraph, Ciavarella comments that *these efforts focusing on roughness remain largely academic.* Since I do not assume that Ciavarella intends to discredit all of linear elasticity with or without adhesion (Hertz, Johnson-Kendall-Roberts, Maugis, etc.) as a mere academic exercise, the comment can only be a criticism of the models for roughness, in particular the random-phase approximation (RPA) defined further below. While I do not dare to contradict his assessment that *I may have indulged myself in this academic exercise in the past!*, it might be wise to only speak for oneself. This also holds for comments such as *tribology remains too complex for quantitative modeling.* As long as ten years ago, the contact mechanics of aluminum-silicon surfaces with quite complex surface topographies deviating substantially from self-affine scaling, could be studied very accurately with computers that were less potent than today's smart-phone processors [15]. Yet, interesting results were found: Small variations in the concentration of the silicon content induced significant changes of stress distribution functions on both the mesoscale and the microscale. Moreover, the tail of the stress distributions showed an exponential decay at large stress rather than Gaussian scaling, which is found for randomly rough surfaces. I mention this to demonstrate my willingness to identify shortcomings in Persson theory or in the assumptions that it is based on.

I feel that the reasons why relatively simple model topographies were used in the Contact-Mechanics Challenge – although it would have been an easy matter to consider an experimentally measured profile instead – are sufficiently well explained in the original literature. Yet our choice keeps drawing criticism beyond Ciavarella's comment. Several people (whose names I forget) have suggested that it would have been more meaningful to base the surface topography on the Weierstrass function. It is sometimes used to model self-affine surface roughness, for example, in Ciavarella's most cited paper [16]. The main reason why I find it to be a poor choice is that it does not look so much like a real surface.

In order to put readers in the position to judge to what extent various computer-generated surfaces resemble reality, Figure 2 shows various cross-sections. They include: (i) a deterministic Weierstrass function, (ii) a randomly rough surface satisfying the RPA, (iii) a sandblasted glass surface, and (iv) a concrete surface consisting of sand particles with binder, which is made smooth at the top during production. Curves (iii) and (iv) are courtesy of Bo Persson. Their measurement is described in Ref. [17]. Since linear elasticity is a scale-free theory, units do not do anything for a qualitative assessment. This is why different profiles were rescaled so that similar features appeared at similar positions in the graph. Readers are invited to look up the literature or take their own line scan with their preferred method to double check what other typical surface scans look like. Ref. [18] summarizes spectra of a wide variety of surfaces, which all look qualitatively similar to the one set up for the Contact-Mechanics Challenge.
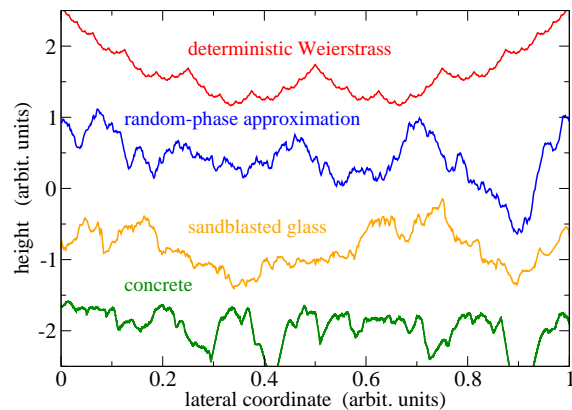

Fig. 2 Line scans of different surface realizations.

There are three main reasons why RPA surfaces look more like real surfaces than Weierstrass does. (i) The phases of $\tilde{h}(\mathbf{q})$ – the complex Fourier transform of a height profile – are uniformally distributed for any surface that is statistically homogeneous (but not necessarily unworn or isotropic). This is why the RPA assumes a uniform distribution as well. In the Weierstrass function, all phases are exactly equal to zero, which turns the profile into a pure cosine transform, i.e., it breaks the translational invariance to the largest possible degree while still showing the usual self-affine scaling of the height-autocorrelation function. The RPA assumes that there is no stochastically relevant correlation between the phases of different $\tilde{h}(\mathbf{q})$ at all, which, certainly can be an approximation. (ii) Real surfaces and the challenge surface are two dimensional, while the Weierstrass function is only a one-dimensional realization. Although two-dimensional generalizations of Weierstrass look intriguing, they appear even more artificial than their one-dimensional versions. (iii) In reality, different $\mathbf{q}$-vectors have equal a-priori weight. This was our main motivation to discretize the wave-vector components on an equidistant grid, leading to a quasi-continuous distribution of $\mathbf{q}$ vectors. The spectrum of

the Weierstrass function is designed such that the spacing between adjacent $\tilde{h}(q)$ peaks increases exponentially with the wave number q. Thus, the Weierstrass spectrum is a discontinuous rather than a quasi-continuous function of q, while any technical surface has a continuous height spectrum. For these reasons, it remains a mystery to me why the study of a Weierstrass profile should add more insight for real systems than that of a profile satisfying the RPA.

While the RPA profile and the sandblasted glass appear rather similar, the concrete surface has some deep troughs, as many other polished surfaces do, which are ignored by any RPA profile. A naive interpretation of Persson theory, or potentially other theories that take the height spectrum as input, is then not meaningful. However, any creative scientist would simply adjust the theory to a given problem and not deem a theory useless, just because he cannot see use or generalize to use it properly. For the given polished surface, two simple possibilities immediately arise. In a first step, the height or even better the height-difference autocorrelation function $C_{\delta h}(\Delta r)$ could be deduced on, say, only the top 50% of the surface and the spectrum be obtained through a Fourier or Hankel transform of $C_{\delta h}(\Delta r)$ in a second step [19, 20]. Alternatively, a true multi-scale method could be used. For example, a boundary-value method solves the problem on a coarse scale and Persson (or some other spectral) theory is applied locally. This would be a procedure similar to FE^2, or, to the strategies [21, 22] pursued by the Carbone group and the Jackson group in the Contact Mechanics Challenge.

The role of the "thermodynamic limit". Ciavarella writes: *Persson's theory is a "thermodynamic limit", but a tribologist may not know what this implies, and [7] is never quite clear about this approximation.* One could state – loosely based on Gertrude Stein [23] – theory is a theory is a theory is a theory, but how can a theory be a thermodynamic limit? Also, I am quite confident that most tribologists can type the words "thermodynamic limit" and "wiki" into a search engine if they do not know that thermodynamics is a theory for large particle numbers. The first sentence in the Wikipedia page on the term "Thermodynamic limit" (Nov 15, 2017) reads *The thermodynamic limit ... is the limit for a large number N of particles.*

In the context of contact mechanics, it should be immediately clear that a large number of particles implies a large number of asperities in contact. In other words, making a theory for the thermodynamic limit is an attempt to predict the contact mechanics of a representative surface element. The questions when a contact is large enough to be considered representative and how to apply Persson theory when finite-size effects come into play are very well discussed in the literature [24] and this work has been cited by Ciavarella. The approach to the thermodynamic limit has also been considered numerically [8, 9, 24] and was found to be quite rapid – as in Persson theory or other RG approaches. It is unclear why Ciavarella nevertheless writes *... never quite clear about this approximation* and also why he objects to the study of representative surface elements in Persson theory but not in his own or other GW-based work?

Final remarks. Ciavarella's comment opens with the assessment that *"Meeting the Contact-Mechanics Challenge" [1] is a very useful and tremendous effort* and closes with expressing his hope that his *comment is a useful contribution to this debate.* Yes, conducting the Contact-Mechanics Challenge was a tremendous effort and I thank Ciavarella for recognizing that. However, because of his comment, I now know that it has not reached the goal that I originally had in mind.

The reason why I set up the contact-mechanics challenge was to create a counter weight to the many, meaningless studies, which are now published, in particular, but not exclusively, in high-impact journals. A journal such as Tribology Letters, in which the editorial board consists of active and knowledgeable scientists, was – and still is – an excellent choice for such an endeavor. The intent was to show that most of the people making big claims in contact mechanics are not in a position to perform real predictions. The hope was that scientists would recognize what approach is reliable and to potentially entice some degree of self reflection.

The fact that Persson – as any other challenge participant – had the courage to make a true prediction on a rather complex problem and that his prediction matched all quasi-exact methods almost flawlessly apparently did not impress Ciavarella. Yet, Ciavarella, who did not contribute to the challenge, judged from a safe distance, *the conclusions are less strong than they seem.* If true predictions and their rigorous tests no longer matter in the sciences, where do they matter?

It seems as though it frequently suffices to write something negative about an undesired theory to get endorsed by a referee – a process, which reminds me of Sokal's hoax, in which he unmasked poor refereeing standards in the social sciences. If a comment failing desirable scientific standards were an accident, it would not be a problem. However, it is anything but a rare event and the Contact-Mechanics Challenge obviously did not succeed in impeding the dissemination of meaningless contributions. Instead, we may expect that more studies will appear, in which conclusions on non-representative surface are falsely claimed to matter for macroscopic systems.

Unfortunately, not only this comment but also other works of Ciavarella appear to be problematic [25]. One example having substantial overlap with the submitted comment is a recent study on the load-separation curves for the contact of self-affine surfaces [26]. Even when reviewers clearly point out obvious deficiancies, editors decide to accept such submissions. In the case of Ciavarella's comment, the editors' motivation may have been to avoid the impression of censorship. Otherwise, the scientific competence and/or integrity revealed in the reviewing and editorial process might have to be asked into question.

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