

Habilitation thesis reviewer's report

Masaryk University	...
Faculty	...
Field of study	.. Visualization
Applicant	name and surname, including academic degrees:
Unit	.. Barbra Kozlíková, PhD
Habilitation thesis (title)	.. Visualization of Biomolecules
Reviewer	name and surname, including academic degrees:
Unit	.. Reviewer: Pere-Pau Vázquez, PhD

Reviewer's report (extent of text up to the reviewer)

Attached to this document

Reviewer's questions for the habilitation thesis defence (number of questions up to the reviewer) ...

Attached to this document

Conclusion

The habilitation thesis submitted by [name and surname of applicant] entitled ["habilitation thesis title"] meets – ~~does not meet~~ the requirements applicable to habilitation theses in the field of [field of study].

In Brno on

19th March 2017

Habilitation thesis reviewer's report

Reviewer information

Name and surnames: Pere-Pau Vázquez Alcocer

Degrees: Engineer in Computer Science, Phd in Software

Field of study: Visualization and Computer Graphics

Habilitation thesis information

Name of the applicant: Barbora Kozlíková

Field of study: Visualization

University: Masaryk University, Brno

Reviewer's Report

1 Contents of the document and methodology

This document contains my habilitation review for Dr. Barbora Kozlíková. Throughout the document, I analyze the different aspects of her CV and I provide as a conclusion my opinion in her validity for obtaining the habilitation.

1.1 Organization of the document

I have written the document divided in three main sections:

- Research CV
- Teaching CV
- Habilitation Thesis

I analyze the three parts independently. However, I give the most value to the research CV, more concretely the list of publications, since these are the outcomes I can value the most. Of course, to have a complete profile, one must be able to publish but also to secure funding, but the information I got for the evaluation is partially in Czech, and some bits are not as complete as would be necessary for a deeper evaluation. For example, and as it will be commented later, the granted projects do not have the information on the amount of budget secured, and the funding agency is not clear to me in some cases (maybe the name belongs to a national institution which is unknown to me). However, in any case, the information I got from the habilitation thesis document serves enough for me to make my evaluation with total confidence.

In the first part, of this report, I evaluate the quality of the research CV. This includes not only publications, but also other merits such as invited talks, external collaborations, and so on.

The second part deals with the teaching CV. Like in the case of the projects commented above, I have not enough information on how complex the teaching can be. As far as I understand, most of the courses seem to be relatively small, but this is not bad by itself, since whether the candidate teaches big courses with 200+ students, where the course responsible must coordinate several other teachers, or the candidate teaches small and simpler courses with 20 students does not usually depend on the candidate, but on the characteristics of the university itself. This will be commented later, but I believe that what I get from the documentation is enough.

Finally, I will briefly elaborate on the habilitation thesis document itself.

1.2 Guidelines

I do not have an idea of the standards followed in the Czech Republic for evaluating a habilitation thesis. So, what I did in order to write the report, is to follow the references I have from the Spain and Catalan quality assessment agencies, who provide detailed guidelines to evaluate the candidates for the different positions in the university in Spain (ANECA: <http://www.aneca.es>) and Catalonia (AQU Catalunya: <http://www.aqu.cat>). In my case, I have taken as reference the guidelines for the evaluation of Associate Professor, which detail the number and quality of publications, as well as the teaching and project funding that has to be obtained to get a positive evaluation.

I also have extensive previous experience in the evaluation of CVs in other regions of Spain, for evaluation institutions analogous to ANECA or AQU, so I am pretty confident that the guidelines I followed are valid.

I have also used my knowledge on how similar procedures are carried out in other countries in the UE, but in this case, I have not access to detailed guidelines.

2 Research CV

In this section I evaluate the information concerning publications, internationalization of the research, collaborations, and so on.

I end this section with a small conclusion on the quality of the research the candidate has developed so far.

1.1 Publications

Dr. Kozlikova has a number of papers published in the most important conferences and journals of the visualization area. Her research covers some theoretical aspects, such as in the papers dealing with the development of the cavity detection. However, in other cases, she also provides more practical solutions to hard and open problems of molecular visualization. I find this fact as very positive, not only because the results of the research may reach to a broader audience, but also because this way, researchers get a deeper understanding of the problems that can be used to find more useful solutions.

It is well known that finding cavities of molecules is an important problem that has been addressed by hundreds of papers. The solution they propose, is not only valid, but they also provide the source code for free. This is remarkable, since one not often sees those large portions of software being provided as open source. It is more common in the visualization area but far less in Computer Graphics.

The candidate has been able (in collaboration of her colleagues, of course) to position CAVER as a well-known software, not only among our community, but also in molecular research. This is notable, because, although the objective has been always to produce interdisciplinary research, coming from a more computer science background sometimes makes it difficult to get the people in other fields to adopt one's software.

The evolution of CAVER into CAVER Analyst is also a good step, since the added functionalities may make the software package as a whole to be adopted by larger communities. Not only this, but as I see in my collaborations with biotechnologists, in molecular science, the researchers are still using a bunch of packages that are quite old and show their age. Although big players are still repositioning themselves and adopting the advanced rendering techniques, it is not surprising to see then products developed by more computer graphics people, such as QtMol or MegaMol (also CAVER) being mentioned more and more in other fields.

This is a gap that I believe the new researchers will overcome, since nowadays it is more common to see interdisciplinary research.

I have gone through the publications, and it is interesting to find that the candidate has covered many areas, from more detailed papers on a certain feature, such as the comparative analysis of secondary structures, to survey papers that broadly describe the state of a field. A researcher does not commonly participate in many of those throughout her career, and Dr. Kozlikova has participated in two in the last two years, both in EuroVis. And in both cases the result is of high quality. I find this an outstanding achievement, since writing such a paper is a service to the community that involves a high amount of work. Even if there are several authors, coordinating them is complex, and the candidate has done this task twice, and has been successful in both cases.

In my opinion, publications the candidate has managed to get so far is more than enough to obtain a habilitation, not only in the number, which is large, but also in the quality. The last years she has been able to publish several papers in the VIS conference, which is the top notch in the visualization area, and several other papers have gone to journals in Biology and Bioinformatics, which proves the importance of her work in related areas such as biotechnology.

1.2 Research trajectory

The trajectory of Barbora Kozlikova has seen a clear evolution, from the beginnings where more hands on work was done, to the current research, where she is leading most of the papers she publishes. Moreover, you can see a clear evolution in the quality of the publications. As usual, the initial publications of the thesis were less ambitious than the ones the candidate is achieving in this point of her career.

I have analyzed the publications in the habilitation, but I have also checked the complete list that appears in the candidate's profile in Google Scholar, which serves to have an overview of somebody's research trajectory over the years. From the profile (where there might be some publications missing), one can count 30+ contributions, and a notable evolution in terms of number and quality in the last 3 years or so.

Since she has been consistently publishing in the top conferences and journals in our area, there is nothing to be said against her trajectory. Moreover, the sustained collaboration with molecular scientists as well as other scientists in several of the most important research centers in visualization in Europe demonstrate her value and her accomplishments. As a result, she has been invited to several research centers to give invited talks, and she is in the moment of her career where her collaborations and international impact is growing.

1.3 Internationalization efforts

One of the aspects that I value the most in every scientist is the ability to publish and collaborate internationally. Everyone may agree that international collaborations are one of the best ways to improve the researcher's career.

When analyzing the CV of the candidate, it is easy to see how a relevant percentage of the papers the candidate has published the last years have one or more co-authors from different countries. This is always positive and enriches the quality of the CV.

From the documentation one can see that the candidate has also been visitor in several institutions (U. Bergen, TU Wien, and U. Postdam). The outcomes are clear in the publication list, so one can only deduce that the visits have been more than fruitful there, so the candidate has made her best to take advantage from the time spent there.

She has also been asked to participate as a reviewer or program committee member in several international conferences and journals. This denotes the fact that the community is also confident on her performance when evaluating peer's works.

Finally, I have also analyzed the amount of citations obtained by her work, both from the information I got in the documentation, and checking Google Scholar. In the documentation, the candidate has been asked to depict the three most relevant contributions, and the paper on CAVER is shown to be as one of the most cited. There are other papers with a number of citations, but I also expect that some of the papers she has recently published (e.g. the state of the art reports) will receive a notable number of citations the following years, because molecular visualization is currently a hot topic in visualization.

1.4 Leadership

Dr. Kozlikova has demonstrated to be a leader in several projects. Besides the coordination of the two State of the Art papers, mentioned earlier, in which there was a number of high profile authors involved, she has also led several research projects.

From what I understand from the documentation (this part is not in English), she has lead at least 6 projects as the main principal investigator, and co-lead another one. Being a young researcher as she is, the number of granted projects is large enough. I want to be prudent here, because there seems not to be documentation on the amount of budget granted, and the magnitude of the projects themselves, except for the duration. When checking the university profile information, it is clear that at least one of them seems to be a national project, and another of the projects lead by the candidate is also international. As I said, I cannot get more information from the documentation or the website, so it is difficult to evaluate the degree of the competition to secure the funding for these projects. But in any case, even if all of those projects were relatively small, I find the achievement of such number of grants good enough if we take into account the position the candidate holds by now, since in many cases one cannot opt to larger funding when the held position is not permanent.

Besides the funding she has obtained, the candidate has also participated in several other research projects, led by other researchers, which is expected, and therefore needs not be commented furthermore.

1.5 Conclusion

In light of my previous analysis of the candidate's research CV, I am confident that she has enough achievements to obtain a habilitation for the position of Associate Professor or equivalent in any European country. The number of papers, projects, and other achievements are more than enough. Moreover, I have no doubt that her CV will improve in the following years, and that she will continue contributing with high quality research to our community.

2 Teaching trajectory

Like in the case of the projects, this part of the documentation is not in English, so I can only trust the translation I obtained from Google Translate, which in any case is consistent with the structure of the documentation.

2.1 Courses

To the best of my knowledge, the candidate has taught a total of 10 different courses from 2007 until now (after checking the web of the university, which has more information in English than in the documentation, I can see that there are even more). Following the guidelines I mentioned earlier, in the procedures of evaluation for the position of Associate

Professor, this represents a good number, even half of them would be enough provided that they were different to each other and imply preparing different materials and documentation. From the titles I understand that the teaching is quite varied since it goes from teaching Java or .NET to Visualization. Moreover, some of the teaching hours seem to be laboratory sessions, and some of them are more classical theory sessions. I believe that this variety in the teaching provides the candidate with enough experience to be a good candidate for the habilitation.

Moreover, from the numbers of students, it seems that the candidate has been the unique responsible of most of the courses, which is important to give the candidate a good view on the overall work that has to be addressed when you have a permanent teaching position in a university.

In my experience, I believe that the number of courses and the variety in them is enough for a positive evaluation. As I said previously, without inside knowledge in the University of Masaryk, it is difficult for me to further analyze this. Moreover, I do not get from the provided documentation any information on whether the courses were set up by the candidate, which would give her extra merits, or she was inheriting courses that had been previously prepared by other professors. I assume that the candidate has followed the typical steps in the case of an inherited course and that she has prepared new materials. I also imagine that the visualization course, which is closer to her profile and where she is the lecturer, is mainly composed by her materials, but I have not had access to them, since they are not publicly available, so I cannot elaborate further.

2.2. Student supervision.

Being a professor not only involves teaching regular courses. On the contrary, it is necessary to perform several kinds of student supervision, from bachelor to PhD thesis. In this aspect, the candidate has also supervised a high number of final projects (31), which is a big number if we compare with the number of students of the courses, and the number of years the candidate has been teaching. This demonstrates her ability to gather students. There is also a number of students doing (or having finished) the PhD. Again, in this case it is not clear to me the rules that guide the university. In many places, a person without a permanent position cannot supervise PhD theses. Even in some places such as Germany, a full professor of a University of Applied Sciences cannot supervise a PhD thesis. So I imagine her case is the same. However, one can see by checking the publications list, that the people appearing in the list of collaborators are actively publishing research with the candidate. This means that she is actively acting as co-supervisor at least. This is even a higher number than expected, given the time when she defended her PhD thesis.

To sum up, and as commented earlier, the candidate has taught a number of different courses, and has participated in them with different tasks, which will provide her the needed overview to supervise future courses in the university. She has also supervised a large number of projects and she is also demonstrating the abilities to supervise PhD theses. This complements the requirements that are expected from a future professor. So, from my point of view, she has enough merits also in this aspect to obtain a positive evaluation.

3 Habilitation thesis

The document of the habilitation thesis is well written. A good introduction to molecular visualization is given, and the outline of the candidate's trajectory is clear. Moreover, the contributions presented, which are a clear continuation and evolution from her PhD thesis are strong and demonstrate the value of the candidate to obtain a habilitation with the standards I think have to be applied.

Since most of her achievements have already been commented when analyzing her research CV, there is little to be said here.

4 Conclusion

As I introduced in the beginning of this document, I have followed the guidelines of the Spanish and the Catalan evaluation agencies to assess the quality of the candidate for the habilitation thesis.

According to the mentioned guidelines, I can only say that the candidate meets all the requirements that would be asked to a candidate for a position of Associate Professor in the Spanish university system.

More concretely, she meets the requirements in the following aspects:

- Number of publications: She has a high number of publications in international events and journals.
- Quality of publications (these are typically measured according to a minimum requirement of journals in the Q1 of the Journal of Citations Reports). The candidate has successfully published in several journals (e.g. IEEE TVGC and CGF) that are considered as high quality in our area. Moreover, some of her publications have appeared as special issues from the VIS conference, the top notch venue all the Scientific Visualization researchers take as reference.
- Number and variety of courses taught: She has taught a wide number of courses, and has had different profiles in them.
- Student supervision: She has supervised a high number of students in several projects going from Bachelor projects to more advanced research collaborations.
- Secure funding: The candidate has obtained a number of grants from the university as well as other national funding agencies.

In conclusion I believe that Dr. Barbora Kozlíková meets the requirements applicable to habilitation theses in the field of visualization and computer graphics.

Questions for the habilitation thesis defense

I do not know how long is devoted to the questions, neither how many questions are typically asked. If I was present at the defense, these are probably the questions I would ask:

- There have been several moves to 3D by the different commercial software vendors. What do you think of moving the visualization to Virtual Reality?
- If you would start your research now, with your current background, would you go for 2D or 3D depictions?
- What technology (either hardware or software) do you believe will have a greater impact, or you are willing to test in molecular visualization in the near future?
- What is the hardest problem you would like to address? Why?
- How would you use perception to improve molecular visualization in 3D?

Conclusion

The habilitation thesis submitted by Barbora Kozlíková entitled Analysis and Visualization of Biomolecules **meets** the requirements applicable to habilitation theses in the field of visualization and computer graphics.

And to certify this I sign this document in Barcelona, the 19th of March, 2017.

Pere-Pau Vázquez, PhD

Associate Professor, Universitat Politècnica de Catalunya, Barcelona