Posudek diplomové práce

Matematicko-fyzikální fakulta Univerzity Karlovy

Autor práce	Bc. Pavel Mikuš		
Název práce	Simulating image formation in an electron microscope by electron tracing		
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Studijní program	Informatika	**Studijní obor**	Počítačová grafika a vývoj počítačových her

Autor posudku	Mgr. Tomáš Iser	**Role**	Vedoucí
Pracoviště	KSVI		

Text posudku:

This diploma thesis deals with the problem of simulating how images are formed in an electron microscope (EM). Solving this problem is important for two reasons: 1) to create a "playground", where users can examine the processes in EM in a virtual environment, and 2) to possibly have fast and reasonably accurate estimations needed in inverse reconstructions.

This problem was already solved before, however, the existing approaches are either naïve and very approximative (the transmittance model), or slow and complicated (the multislice model). This thesis presents a different way of looking at the problem: through the eyes of particle tracing in heterogeneous volumes, where the particles we trace are electrons, and the heterogeneous volume are the molecules (atoms) forming the sample in the microscope. The author explained the electron-matter interactions that may occur and described formulas for electron scattering, which they used in the corresponding radiative transfer equation. Then, appropriate Monte Carlo estimators were derived that allow solving it in a reasonably fast way that was implemented in C++/CUDA. By comparing the simulated images to real data, it was shown that the method is indeed capable of achieving very high accuracies, despite approximations in the estimator's design.

From a formal standpoint, the work was written in good English with a reasonable typography, mostly clear formulas and equations, and many illustrative figures that were provided for better comprehension. A few typographical and stylistic improvements could be made, e.g., in tables, that sometimes feel too "bulky", or figures, that combine many different styles and do not feel unified throughout the paper. The structure and length also seem adequate. My only main criticism there would go to references: I think a bit more time could be spent on discussing related approaches, radiative transfer simulations in physics, or the fundamental differences of particle vs. wave-based methods.

From a supervisor's point of view, I would like to note that the author faced many challenges when working on the thesis, and these had to be solved or worked around, such as the necessity to solve large Fourier transforms during interactions; the fact that scattering coefficients are not known, hence mean free paths must be approximated from scattering cross sections and chemical compositions; or the fact that the typical mean free paths of electrons are extremely long, which resulted in a lot of noise.

Solving these and many more challenges showed that the author is not afraid of tackling problems and designing solutions. I was overall impressed by the author's maturity in setting and following his own deadlines, organizing meetings with me, periodically updating me on

the work's progress, preparing a presentation for a seminar, and generally handling the project management very well and with high interest.

For these reasons, I do recommend the thesis for defense and believe the candidate will be a valuable addition to any engineering or research team he will join after finishing his studies.

Práci doporučuji k obhajobě.

Práci nenavrhuji na zvláštní ocenění.

Pokud práci navrhujete na zvláštní ocenění (cena děkana apod.), prosím uveďte zde stručné zdůvodnění (vzniklé publikace, významnost tématu, inovativnost práce apod.).

Datum 25.01.2021 **Podpis**