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A Molecular Dynamics and Transition Path Sampling study

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Appendix: Evaluating Science

Technological progress has been identified as the main factor boosting economic growth in the 20th century, as argued by the 1987 economy Nobel prize winner Robert Solow [1, 2]. Economists estimate the contribution of science to economic growth has been 20%-60% return on investments. Taking the example of basic research in the US in the post-war period, science has been primarily boosted by government funding. This model of primarily public funded research has been criticized during and after the 1990s by the New Public Management (NPM) administration of universities and research institutes.

According to NPM, the public sector would turn more efficient and effective under the evaluation and control by market forces [3]. This led to a severe change in the orientation of science and research away from primarily facilitating basic research, and towards an output performance strategy. According to a Dutch education ministry policy paper [4], valorization was introduced to describe the third main task of universities, the transfer of knowledge to society. Nowadays, NWO grants research proposals more favourably if they involve research with commercial benefits. Therefore, the question raised is whether this trend allows science to make progress and whether science should impact and benefit society. I will try to argue on how valorization as done nowadays often impinges on societal benefits and on science itself.

First of all, getting more and more driven by commercial needs, science poses low risk goals to itself, thus solving only short-term problems. However, basic research investigating different possible theories, involves high risk. During the 1920s, before Heisenberg introduced the uncertainty principle, Pauli wrote to a friend "For now, physics is again in confusion. I find physics too difficult for me and I would rather be an actor". A few months later and after Heisenberg's paper, he wrote again to his friend saying "The type of mechanics brought up by Heisenberg gave me hope and joy for life". Scientific breakthroughs as the above signify the complex way science evolves, often without guarantee that a hypothesis will work, leaving the scientific debate open. Imagine what a tremendous mistake it would have been if Werner Heisenberg lived in the present having been unable to get a research grant only because his proposal wasn't societally relevant or commercial enough.

Secondly, a crucial element of valorization is the existence of intelectual property rights (IPs). By introducing IPs, scientific knowledge and output is no longer freely available for sharing within the scientific community. This growing protection of science infrastructure and services endangers science, and hinders innovation, as scientists or innovators might find it costly to use protected material of other Institutes / Publishing houses / companies [5]. Thirdly valorization, introduces a tension between

principles. Scientists are made responsible to argue about the societal relevance of their research, thus altering their role from scientists having to solve basic problems to delegates of governments having to primarily deliver scientific products [6].

Notwithstanding the dangers of society and market driving research, I do believe that challenges entailed in the Millennium Development Goals (MDGs) [6] such as reduction of poverty, hunger and diseases are highly important for humankind. Therefore, public universities and institutions should indeed expand the definition of valorization towards societal goals, which are often no-commercial. Scientific knoweldge and output should be openly shared and communicated.

However, science is not only about solving societal needs. It has autonomy and its own pace. According to Thomas Khun [7], conventional science is about solving puzzles, accumulating knowledge and making step-by-step progress which often leads to new technologies. However, the inability to make progress on these puzzles creates crises of existing theories and sometimes leads to a change of "epistemological paradigm", followed by a new theory. Such a change of paradigm has been Einstein's theory on general relativity which generalized special relativity and Newton's law of gravitation, providing a unified description of gravity as a geometry of space and time.

To conclude, science can have societal impact when not seen as a scientific factory. The possibility it gives to explore unexplored territories, the hope it creates to discover existing order in nature, the feeling of being useful, the curiosity to test the validity of established knowledge, are all virtuous driving forces. Once these ingredients are there, science has proved it can achieve breakthroughs with an increased societal impact.

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