Ideas in the History of Nano/Miniaturization and (Quantum) Simulators: Feynman, Education and Research Reorientation in Translational Science Francisco Torrens¹ and Gloria Castellano²

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Cultural history of nanominiaturization, computing, quantum computing and simulating is necessary to comprehend human character and place it in the whole of living beings. Ideas in the history of physics by Feynman, *etc.* are valued by the questions that generate. A series of questions, answers and hypothesis introduces the nature of the history of nanominiaturization, providing facts. Nanotechnology adds a third dimension to the periodic table of the elements. Thinking about computers was useful. It must do with learning computers possibilities and physics potential. Provisional conclusions follow. (1) Nature (space–time) is not classical but discrete; quantization is a different kind of mathematics. (2) Nanomaterials differ from conventional ones because of large surface-to-volume ratios and quantum effects. (3) Feynman predicted: (a) in the nanoworld, one has a lot of things that would happen that represent opportunities for design; (b) other way to simulate the probabilistic nature is by a computer, which itself be probabilistic. (4) Problems are temperature and isolation. (5) Advances exist in low-temperature materials and high-energy physics; promises, in superconductivity. (6) Computing possibilities tell people about computer rules and physics. (7) Philosophers work better if they are interested in the data that scientists unveil. (8) Researchers should not be afraid to transcend cultural boundaries in search for the truth.

Keywords: Nanoworld research, Nanolaboratory, Nanophysics, Nanochemistry, Nanomaterial, Nanoprobe, Nanosensor, Nanotechnology, Quantum computing, Computing, Technology, Probability, Determinism, Cultural history of physics, Philosophical discussion, Culture.

INTRODUCTION

The seminal idea of nanotechnology was first proposed by Feynman (1959) in his visionary conference entitled *There is plenty of room at the bottom*, in which he discussed the importance *of manipulating and controlling things on a small scale*, and described how physical properties of nanomaterials differ significantly from those of conventional ones because of large surface-to-volume ratios and quantum effects [1]. What then could to someone seem the idea of a lunatic (it was not till 1965 that he received the Nobel Prize in Physics) nowadays it is a scientific field with a vertiginous development; in fact, the concept of *nanotechnology* transcended from the scientific subjects to be also discussed in the political, social and business ones. A series of questions (Qs) and hypothesis (H) on nanolaboratories follow.

Q1. Why is the field of nanotechnology and nanoscience important?

Q2. What is really new?

Q3. How can one do research in the nanoworld?

Q4. How does one make a nanomaterial?

Q5. How are its novel properties exploited for a range of current and future technologies?

H1. Nanotechnology adds a third dimension to the periodic table of the elements (PTE).

The cultural history of nanominiaturization and quantum simulators (computers) turned out to be essential to understand human nature and place it in the whole of living beings. A series of Qs were raised to introduce miniaturization on the nanoscale and quantum simulators.

Q6. Is the nanoworld either a limitation or a lot of new things that would happen that represent completely new opportunities for design?

Q7. Is it better to simulate the probabilistic nature by either a quantum computer or a quantum simulator?

The discovery of computers and thinking about them turned out to be useful in branches of human reasoning; *e.g.*, people never really understood how lousy their comprehension of languages

was, theory of grammar, psychology, etc. until they tried to make a computer that would be able to understand language, etc. The rule of simulation is that the number of computer elements required to simulate a large physical system is only to be proportional to the space-time volume of the system. The phenomena of field theory are imitated by occurrences in solid state theory (analysis of a latticework of crystal atoms), where *atom* is just a point that has numbers associated with it via quantum-mechanical rules and *quantum number* is just a constant of motion. Many nanomaterials with extraordinary thermal, mechanical, optical, electrical and magnetic properties are promising in many fields, e.g., biomedical, drug delivery systems and cancer therapy, energy storage devices, composites fillers, nanoprobes/sensors and catalysts. Although without considering quantumnonlocality developments, quantum-computation idea was first considered by Feynman in a course on computation (Caltech, 1981–1986), with which notes a monograph was produced [2]. The sixth chapter treats on quantum computation, which deals with the central element of quantum computation: using that *quantum superposition* allows handling states in more than two situations (bits either 1 or 0), giving rise to quantum bits (qubits). The first realistic proposal for building a quantum computer was made by Cirac and Zoller, then members of the Institute for Theoretical Physics at the University of Innsbruck [3]. Their scheme consisted of a set of N cold ions, confined by a light amplification by stimulated emission of radiation (laser), that would form a system stable enough to produce a quantum computer.

In earlier publications, fractal hybrid-orbital analysis [4,5], resonance [6], molecular diversity [7], PTE [8], law, property, information entropy, molecular classification [9] and simulators [10] were reviewed. In the present report, Qs were raised on the nature of nanominiaturization cultural history and provide facts. Computational simulating physics was examined. Nature is quantum mechanical and problem is quantum-physics simulation. Necessity of a reorientation of translational-science research is discussed. Reorientation is performed by bench-guided reverse engineering; in a society, by culture-guided reverse engineering.

THERE IS PLENTY OF ROOM AT THE BOTTOM

Feynman raised the following Qs on problem of manipulating and controlling things on a small scale.

Q1. What are the strange particles?

Q2. What is miniaturization?

Q3. How far has it progressed today?

Q4. In 2000, when one look back at that age, one will wonder why was it not until 1959 that anybody began seriously to move in this direction?

Q5. Why cannot one write the entire 24 volumes of the Encyclopaedia Brittanica on the head of a pin?

Q6. Is it possible to reduce in size all the writing in the Encyclopaedia by 25 000 times?

Q7. How would one read it?

He raised the following Qs on how one writes small.

Q8. How does one write small?

Q9. Will an electron beam etch away a metal it is run long enough?

Q10. What would happen if one prints all the books of interest in the world (say, $24 \cdot 10^6$ volumes) down at the scale we have been discussing?

Q11. How much space would it take?

Q12. What would our librarian at Caltech say, as she runs all over from one building to another, if I tell her that, ten years from now, all information that she is struggling to keep track of (120 000 volumes) can be kept on just one library card?

He raised the following Q on information on a small scale.

Q13. How could it be that, in the tiniest cell, all information for the organization of a complex creature, *e.g.*, humans, can be stored?

He raised the following Qs on better electron microscopes.

Q14. If one has written in a code, with $5 \times 5 \times 5$ atoms to a bit, how could one read it today?

Q15. What good would it be to see individual atoms distinctly?

- Q16. Do you know the reason you fellows are making so little progress?
- Q17. What are the most central and fundamental problems in biology today?
- Q18. What is the sequence of bases in the deoxyribonucleic acid (DNA)?
- Q19. What does it happen when one has a mutation?
- Q20. How is the base order in DNA connected to the order of amino acids (AAs) in the protein?
- Q21. What is the structure of the ribonucleic acid (RNA)?
- Q22. Is it single-chain or double-chain?
- Q23. How is it related in its order of bases to DNA?
- Q24. What is the organization of the microsomes?
- Q25. How are proteins synthesized?
- Q26. Where does RNA go?
- Q27. How does it sit?
- Q28. Where do the proteins sit?
- Q29. Where do AAs go in?
- Q30. In photosynthesis, where is the chlorophyll?
- Q31. How is it arranged?
- Q32. Where are the carotenoids involved in this thing?
- Q33. What is the system of the conversion of light into chemical energy?
- Q34. Can the physicists do something about synthesis?
- Q35. Is there a physical way to synthesize any chemical substance?
- Q36. Why must the field be symmetrical?
- Q37. Is there no way to make the electron microscope more powerful?

He raised the following Q on the marvellous biological system.

Q38. Can one manufacture an object that manoeuvres at the cellular level?

He raised the following Qs on miniaturizing the computer.

Q39. How to miniaturize the computer on a small scale in a practical way?

Q40. Why cannot one make them small, make them of little wires, little elements?

He raised the following Qs on miniaturization by evaporation.

Q41. How can one make a small computer?

Q42. What kind of manufacturing process would one use?

Q43. Why cannot one manufacture the small computers somewhat like one manufactures the big ones?

Q44. Why cannot one drill holes, cut things, solder things, stamp things out, mould different shapes all at an infinitesimal level?

Q45. What are the limitations as to how small a thing must be before one can no longer mould it?

Q46. How many times when one is working on something frustratingly tiny like his wife's wrist watch, has one said to himself, *If I could only train an ant to do this?*

Q47. What are the possibilities of small but movable machines?

Q48. What are the problems of making an infinitesimal machine?

He raised the following Qs on problems of lubrication.

Q49. What would be the utility of such machines?

Q50. Who knows?

- Q51. How does one make such a tiny mechanism?
- Q52. How many washers can one manufacture on one lathe?

He raised the following Q on a hundred tiny hands.

Q53. Where is one going to put 10^6 lathes that one is going to have?

He raised the following Qs on rearranging the atoms.

Q54. Ultimately (in the great future), can one arrange the atoms the way one wants?

Q55. What would happen if one could arrange the atoms one by one the way one wants them?

Q56. What could one do with layered structures with just the right layers?

Q57. What would the properties of materials be if one could really arrange the atoms the way one wants them?

Q58. Is it possible to emit light from a whole set of antennas, like one emits radio waves from an organized set of antennas to beam the radio programs to Europe?

He raised the following Qs on atoms in a small world.

Q59. How to synthesize absolutely anything?

Q60. How would it be, in principle, possible for a physicist to synthesize any chemical substance that the chemist writes down?

Q61. Who should do this?

Q62. Why should they do it?

He foresaw that when one gets to the small world, one has a lot of new things that would happen that represent completely new opportunities for design.

SIMULATING PHYSICS WITH COMPUTERS

Feynman raised the following Qs on the problem of simulating physics with computers [11].

Q1. What are the possibilities of computers?

Q2. What are the possibilities in physics?

- Q3. Have people something to learn about physical laws?
- Q4. What kind of computer is people going to use to simulate physics?
- Q5. Can physics be simulated by a *universal computer*?
- Q6. What kind of physics is people going to imitate?
- Q7. What kind of simulation do people mean?
- Q8. How might one modify a physical law?

Q9. One is not objecting to the fact that a physical law is anisotropic in principle, but how anisotropic is it?

He raised the following Qs on simulating time.

- Q10. Is there a way of simulating time, rather than imitating it?
- Q11. If a function depends on *all* the points both in the future and the past, what then?

Q12. If a general kind of computer were laid out, is there in fact an organized algorithm by which a solution could be laid out, *i.e.*, computed?

Q13. How would one lay out numbers so that they automatically satisfy an equation?

Q14. Are there circumstances where one gets functions for which one cannot think, at least right away, of an organized way of laying it out?

Q15. Does not this reduce to the ordinary boundary value, as opposed to initial-value type of calculation?

He raised the following Qs on simulating probability.

Q16. Is there no real problem in understanding the worldview that quantum mechanics represents?

Q17. Is not one sure no real problem exists?

Q18. Can one learn anything from asking this question about computers simulating probability (about this may or may not be mystery as to what the worldview of quantum mechanics is)?

Q19. Is there any other way to simulate a probabilistic nature without calculating the probability?

Q20. What kind of simulation can one have?

Q21. Is an imitator, not doing the same thing as nature, no good?

Q22. How does one know what the probability is?

Q23. How does one expect to predict it with a computer?

Q24. Can one imitate *nature* (quantum mechanics) with a local probabilistic computer?

Q25. How does it behave in a local region?

Q26. How can one simulate with a computer the quantum-mechanical effects?

Q27. How can one simulate quantum mechanics?

Q28. Can one say either let the computer itself be built of quantum-mechanical elements that obey

quantum-mechanical laws or let the computer still be the same kind that one thought of before?

Q29. Can one imitate this situation?

He raised Qs on quantum computers and universal quantum simulators (cf. Fig. 1).



Fig. 1. A quantum simulator.

Q30. Can one do it with a new kind of computer (a quantum computer)?

Q31. What is the universal quantum simulator?

Q32. If one had discrete quantum systems, what other discrete quantum systems are exact imitators of it?

Q33. And is there a class vs. which everything can be matched?

Q34. If one wrote a Hamiltonian that involved only the operators *annihilate*, *create*, *number* and *identity*, locally coupled to corresponding operators on the other space–time points, could one imitate every quantum-mechanical system that be discrete and have a finite number of degrees of freedom?

Q35. Could Fermi particles be described by such a system?

He raised Qs on quantum systems being probabilistically simulated by a classical computer.

Q36. The hidden-variable problem. Can a quantum system be probabilistically simulated by a classical universal computer, in other words, a computer that will give the same probabilities as the quantum system does?

Q37. Can one make a cellular automaton, or something, imitate with the same probability what nature does, where one is going to suppose that quantum mechanics be correct, or at least after one discretizes space and time it be correct, and see if one can do it?

Q38. What properties does Wigner function *W* have that are analogous to an ordinary probability? Q39. Can one make a device that simulates *W*?

Q40. In a quantum system represented by spin-1/2 objects one can find four numbers, four *probabilities* $\{f_{++}, f_{+-}, f_{-+}, f_{--}\}$ that act just like probabilities to find things in the state in which both symbols are up, one is up and one is down, *etc.*, what is the probability that both indices be positive?

Q41. What is the probability that the two indices be the same?

Q42. What is the probability that there is no match between the indices?

He raised the following Qs on negative probabilities.

Q43. Is it a probability for correlated possibilities?

Q44. Can one imitate a quantum-mechanical equation with a probabilistic computer?

Q45. How to simulate probabilities that would have to go negative?

He raised the following Qs on polarization of photons and two-state systems.

Q46. Einstein–Podoslky–Rosen paradox. Why negative *probabilities* cannot be avoided, or at least that one has some sort of difficulty?

Q47. What does it happen in an experiment of separation into two polarized beams?

Q48. What does it happen in an experiment of separation into four polarized beams?

He raised the following Qs on two-photon correlation experiment.

Q49. How would it have to be for a *local* probabilistic computer?

Q50. How do the photons go?

Q51. Why is that a formula cannot reproduce the quantum results if probabilities are real, although

it is easy if they are *probabilities* (negative for some conditions)?

Q52. What probability do two observers get the same result with?

Q53. What is the chance that two observers get the same result?

Q54. What other possibilities are to the kind of logic of quantum mechanics?

Q55. What is the origin of the probabilities in quantum mechanics?

Q56. Philosophical Q1 (PQ1). Is it somehow that one is correlated to the experiments that one does, so that the apparent probabilities do not look like they ought to look if one assumes that they are random?

Q57. PQ2. Cannot one invent a different point of view than the physicists have had to invent to describe quantum mechanics?

Q58. PQ3. Is there some other way out?

Q59. PQ4. Can one imitate an experiment with a device that is going to produce the same results, and that will operate locally, and one tries to invent some kind of way of doing that, and if one does it in the ordinary way of thinking, one finds that one cannot get there with the same probability?Q60. PQ5. Is there any meaning to Q of whether there is free will or predestination?Q61. PQ6. Is it possible to construct a test in which the prediction could be reported to the observer, or instead, have the ability to represent information already been used up?

Q62. PQ7. How to think in these new ways?

He foresaw that the other way to simulate the probabilistic nature is by a computer, which itself be probabilistic.

CLASP: COMMON LISP VIA LLVM/C++ FOR MOLECULAR METAPROGRAMMING

Schafmeister's goal is to build molecules as easily as he can write software; specifically he wants to build molecules that could do things, *e.g.*, go into the body and fix things (*cf.* Fig. 2) [12]. Inspired by Feynman's 1959 talk in which Feynman proposed building machines on a molecular scale, which were atomically precise, where one knows where every atom is in space, he went into biophysics, where he made proteins and solved crystal structures of proteins, and from there into chemistry. Schafmeister raised the following questions on CLASP.

Q1. How has he spent four years developing software to design these molecules?

Q2. Why would not the usual molecular design programs work?

Q3. How did he need a language that already knew the chemical functionality he needed?

Q4. How did he need to be able to look at a million molecules at a time instead of looking at one molecule at a time?

Q5. How difficult is it to write in C++?

Q6. How did he start scripting with Python?

Q7. How did he finally find the answer in writing a new Common LISP program that he calls CLASP?

Q8. Beyond the current and near-term applications of his promising spiroligomers, is CLASP the basis for a new software architecture for computational chemistry and design?



Fig. 2. Christian. Schafmeister Google Tech Talk June 10, 2015.

DISCUSSION

The discovery of computers and thinking about them turned out to be useful in branches of human reasoning; *e.g.*, people never really understood how lousy their comprehension of languages was, theory of grammar, *etc.*, until they tried to make a computer that would be able to understand language. People attempted to learn about psychology endeavouring to understand how computers work. The PQ1–7 exist about reasoning and relationship, observation and measurement, *etc.*, which computers stimulated people to think about anew, with new types of thinking. The computer-type

of thinking would give people some new ideas, if any be really needed. The possibilities of computation are a subject because they tell people something about computer rules and *might* inform them a little concerning physics. Nature is not classical, dammit, and if one wants to make a simulation of nature, one should better make it quantum mechanical, and by golly it is a wonderful problem, because it does not look so easy. Complex systems are difficult to simulate. Quantum systems are even more hard to imitate. A possible solution is *via* quantum simulators (atoms in optical nets, trapped ions). Probably, it will never be done with classic computers. Experiments in many laboratories showed that it was achieved to do simulations, but two problems appeared: temperature and isolation. They showed applications in low-temperature materials and high-energy physics. Feynman foresaw that: (a) when one gets to the small world, one has a lot of new things that would happen that represent completely new opportunities for design (1959); (b) the other way to simulate the probabilistic nature is by a computer, which itself be probabilistic (1982). The big application, however, of Schafmeister's molecular metaprogramming (via a matter compiler) will be to make proteins that do specific things: catalysts, antibodies, channels, etc.; in particular, catalysts (molecules that make other molecules) so that ultimately he could use the catalysts to make his building blocks instead of needing to synthesize chemically them. Bootstrapping the technology in this way would make it inexpensive.

Figure 3 shows a scheme of the reorientation of research in translational (marketable) science.



Fig. 3. Schematic representation of the reorientation of research in translational science. Figure 4 shows research reorientation in translational (marketable) science in a society.



Fig. 4. Schematic representation of the reorientation of research in translational science in a society.

CONCLUDING REMARKS

From the present questions, answer and hypothesis the following remarks can be drawn.

1. It is important whether one's research field becomes fashionable.

2. Nature is not classical.

3. Physical properties of nanomaterials differ significantly from those of conventional ones because of large surface-to-volume ratios and quantum effects.

4. Feynman foresaw that: (a) when one gets to the small world, one has a lot of new things that would happen that represent completely new opportunities for design (1959); (b) other way to simulate the probabilistic nature is by a computer, which itself be probabilistic (1982).

5. Some advances are expected in quantum chemistry, e.g., superconductivity, etc.

6. The possibilities of computation are an interesting subject because they tell people something about computer rules and *might* inform them a little concerning physics.

7. Know thyself! Although philosophers continue to be necessary, they will perform better their essential work if they would be more interested in the relevant data that scientists unveil.

8. The outcome and implications of this report are that there should be no indication of prejudice and enmity in a literary work, and that researchers should not be afraid to transcend cultural boundaries in search for the truth or present the view of the *other* objectively.

9. Physics continues to make important contributions that make a difference to everyone's life; *e.g.*, quantum manipulations with applications to computing. However, the really exciting possibilities will be those we have not yet imagined.

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REFERENCES

1. R. P. Feynman, There is plenty of room at the bottom, *Caltech Eng. Sci.*, 23 (1960) 22-36.

2. R. P. Feynman, *Feynman's Lectures on Computation*, A. J. G. Hey and R. W. Allen, Eds., Addison-Wesley, Reading, MA, 1996.

3. I. Cirac and P. Zoller, Quantum computations with cold trapped ions, *Phys. Rev. Lett.*, **74** (1995) 4091-4094.

4. F. Torrens, Fractals for hybrid orbitals in protein models, *Complexity Int.*, **8** (2001) torren01–1-13.

5. F. Torrens, Fractal hybrid-orbital analysis of the protein tertiary structure, *Complexity Int.*, submitted for publication.

6. F. Torrens and G. Castellano, Resonance in interacting induced-dipole polarizing force fields: Application to force-field derivatives, *Algorithms*, **2** (2009) 437-447.

7. F. Torrens and G. Castellano, Molecular diversity classification *via* information theory: A review. *ICST Trans. Complex Syst.*, **12**(10–12) (2012) e4–1-8.

8. F. Torrens and G. Castellano, Reflections on the nature of the periodic table of the elements: Implications in chemical education, in: *Synthetic Organic Chemistry*, Eds. J. A. Seijas, M. P. Vázquez Tato and S.-K. Lin, MDPI, Basel, Switzerland, 2015, Vol. 18, pp. 8–1-15. 9. M. V. Putz (Ed.), *The Explicative Dictionary of Nanochemistry*, Apple Academic–CRC, Waretown, NJ, in press.

10. F. Torrens and G. Castellano, Reflections on the cultural history of nanominiaturization and quantum simulators (computers), in: *Sensors and Molecular Recognition*, Eds. N. Laguarda Miró, R. Masot Peris and E. Brun Sánchez, Universidad Politécnica de Valencia, València, Spain, in press.

11. R. P. Feynman, Simulating physics with computers, Int. J. Theor. Phys., 21 (1982) 467-488.

12. C. Schafmeister, Clasp: Common Lisp using LLVM and C++ for Molecular Metaprogramming: Towards a Matter Compiler, Google Tech Talk, June 10, 2015.