Simulating Physics with Computers

Richard P. Feynman

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Richard P. Feynman
1918-1988

- MIT (B.Sc.)
  Princeton (Ph.D., research assistant),
  Manhattan Project (atomic bombs),
  Cornell (professor),
  Caltech (professor)

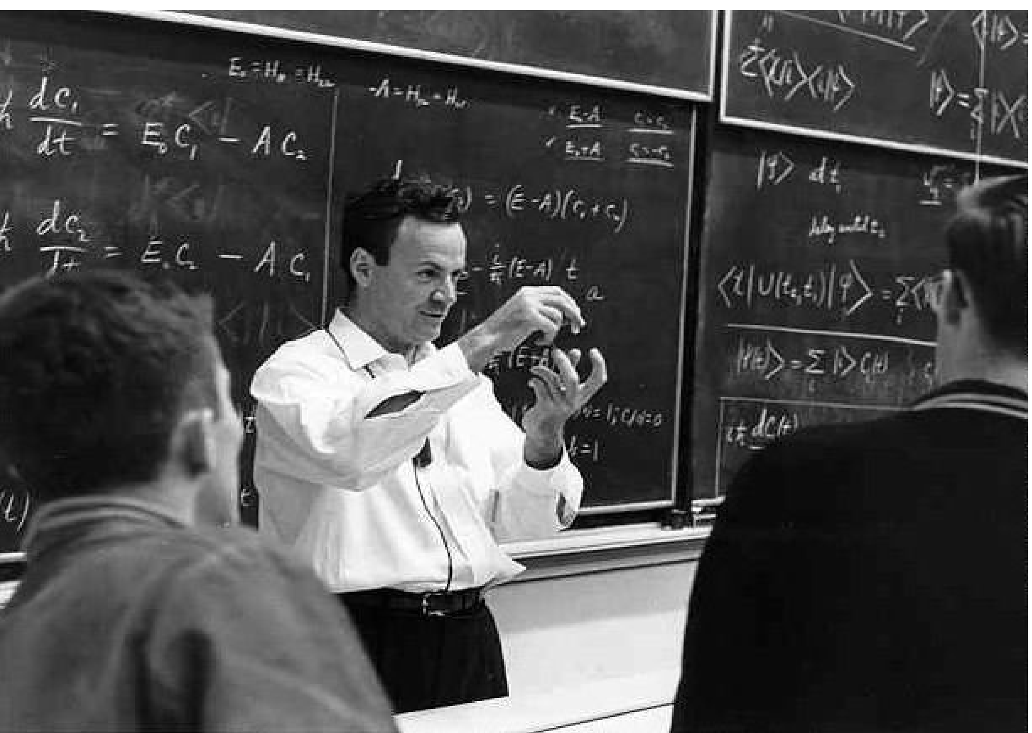
- Quantum electrodynamics (Nobel prize in 1965),
  superfluidity,
  weak nuclear force,
  quark theory

- Famous hobbies: drumming (including a Samba band in Copacabana), safecracking, nude painting for Pasadena massage parlor, space shuttle disaster investigation...

Richard P. Feynman: educator

"A lecture by Dr. Feynman is a rate treat indeed. For humor and drama, suspense and interest it often rivals Broadway stage plays. And above all, it crackles with clarity. If physics is the underlying 'melody' of science, then Dr. Feynman is its most lucid troubadour"

— Los Angeles Times science editor, 1967



Richard P. Feynman: author

- Numerous textbooks / lecture transcripts
  - Feynman Lectures on Physics
  - Feynman Lectures on Computation
  - The Character of Physical Law
  - Quantum Electrodynamics
  - Statistical Mechanics
  - QED: The Strange Theory of Light and Matter
  - ...
- Popular books
  - Surely You're Joking, Mr. Feynman!
  - What Do You Care What Other People Think?
  - ...

Background (1981)

- Quantum theory has matured (to the extent relevant here)
- Computer science is up and running
- Computers have been used extensively for physical computation
- Recently understood links between physics and computation:
  - Maxwell's Daemon: relation between irreversibility in computation and thermodynamics [Landauer 1961][Penrose 1970][Bennett 1982]
  - Universal reversible computation and equivalence to general computation [Bennett 1973][Toffoli 1980]
  - Realization of (classical) Turing machine under quantum formalism [Benioff 1980]
  - *which spurs...*

1st conference on Physics and Computation, MIT, 1981

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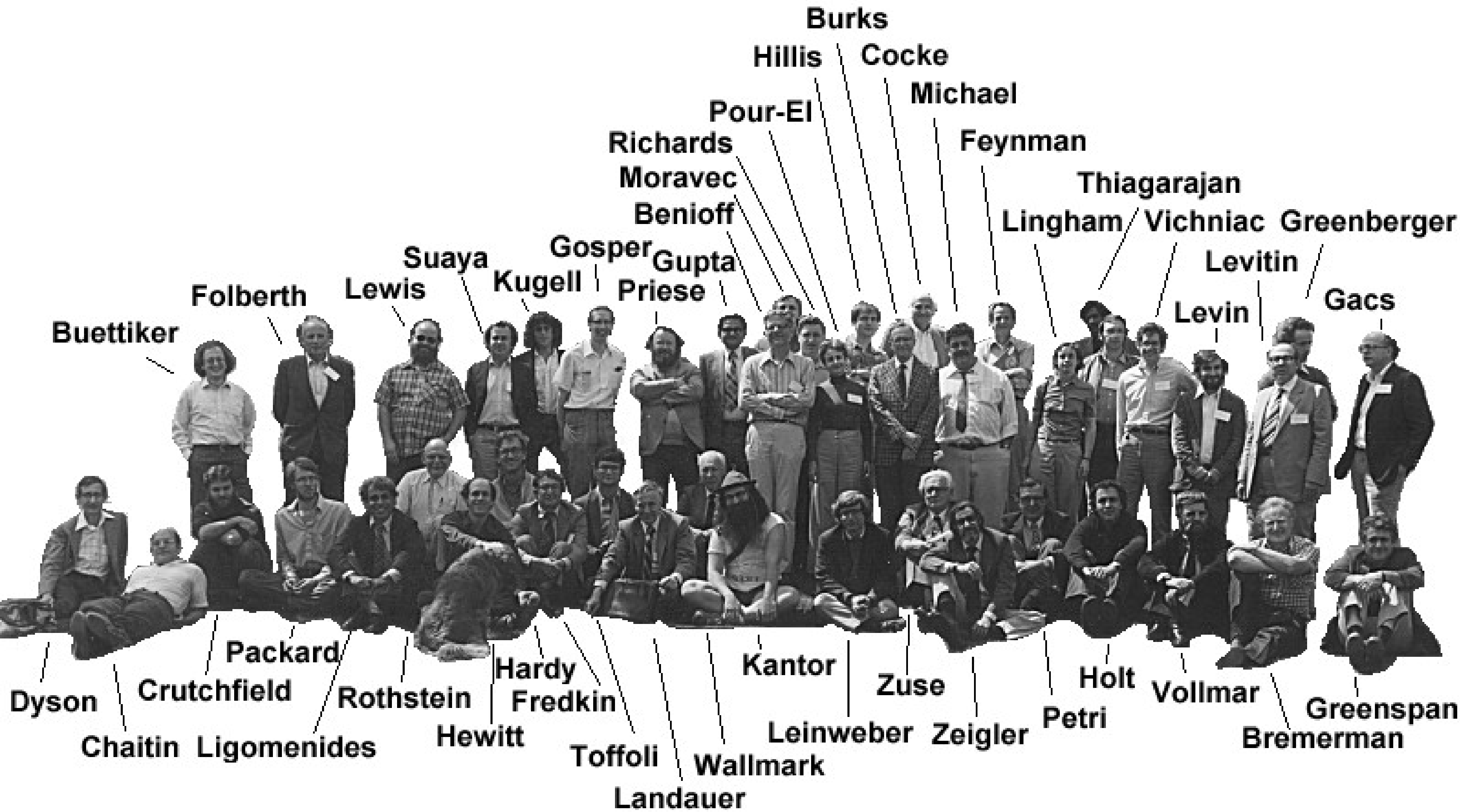

Simulating Physics with Computers
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Keynote talk, 1st conference on Physics and Computation, MIT, 1981
(International Journal of Theoretical Physics, 21: 467–488, 1982)

1. Can classical physics be simulated by a classical computer?
2. Can quantum physics be simulated by a classical computer?

   Classical vs. quantum computational separation

3. Can physics be simulated by a quantum computer?

   Quantum computers

4. Can a quantum simulation be universal?

   Quantum computation theory

“Simulating” physics?

- Inherent part of <u>using</u> physics in other sciences and in technology
- Inherent part of <u>doing</u> physics:
  - Connection between theory and experiment
  - Derivation of known quantities from first principles
  - Identifying deficiencies in the theory (e.g., diverging integrals)
  - Developing interpretations of the theory and conceptualizations of its implications (e.g., Feynman diagrams)

- Computation lead to breakthroughs in linguistics, psychology, logic. Apply “computer-type thinking” to physics too.

(Meanwhile, behind the Iron Curtain...)

- R. P. Poplavskii, *Thermodynamical models of information processing* (in Russian), Uspekhi Fizicheskikh Nauk, 115:3, 465–501, 1975
  - Computational infeasibility of simulating quantum systems on classical computers, due to superposition principle
- Yuri I. Manin, *Computable and uncomputable* (in Russian), Moscow, Sovetskoye Radio, 1980
  - Exploit the exponential number of basis states.
  - Need a theory of quantum computation that captures the fundamental principles without committing to a physical realization.

Simulation requirements

- Exact
  “The computer will do exactly the same as nature”
  Dismisses “numerical algorithms” which yield an “approximate view of what physics have to do”.
- Linear size
  Number of computer elements required for simulation a physical system is proportional (!) to the space-time volume of the physical system.
- Locality
  No long wires (equiv., non-zero propagation delay).

1. Can classical physics be simulated by a classical computer?

Discretization

- Problem: space and time are continuous, but a (classical) computer is discrete.
- Solution: assume/hope/pretend that the laws of nature are discrete at a level sufficiently fine that no current experimental evidence is contradicted.
- Note: discretization ≠ quantization.

Simulating time

- Classical physics is causal, so we can simulate the system's time evolution step by step.
- But then “the time is not simulated at all, it is imitated in the computer”.
- Alternative computational model, where each cell in a space-time computational mesh is a function of its neighbors (both past and future).
- Wonders about classical algorithms for solving this constraint-satisfaction problem...
- **?!**

Simulating probability: explicitly

- How to deal with probabilistic laws of nature (e.g., quantum mechanics)?
- Explicit: the simulation outputs the probability of every outcome
- Problem: discretized probabilities can't be <u>exact</u>.
- Problem: with *R* particles and *N* points in space, a configuration of the physical system contains $\sim N^R$ probabilities. <u>Too large</u> to store (explicitly) in a computer of size $O(N)$.
- “We can't expect to compute the probability of configurations for a probabilistic theory.”
- Roughly: claiming $\#P \neq P$ or $\#P \neq ZPP$
- (Implicit representations and time/space tradeoffs are not discussed.)

Simulating probability: implicitly

- Implicit: the simulation outputs each a (destination of) each outcome with correct probability.
- “Probabilistic simulator of a probabilistic nature.”
- Monte Carlo computation:
  To get a prediction, run the simulator many times and compute its statistics. You will get the same accuracy as in measurements of the physical system.

- **?!**
  - But if an approximation vs. resources trade-off is allowed, why can't it allowed for the explicit simulator?
  - The probability discretization problem remains (up to a polymomial factor)

2. Can quantum physics be simulated by a classical computer?

Q&A

- “Can a quantum system be probabilistically simulated by a classical (probabilistic, I assume) universal computer? In other words, a computer which will give the same probabilities as the quantum system does.”

  (with discretized time and space, and implicit output)

- “The answer is certainly, 'No!' This is called the hidden-variable theorem: It is impossible to represent the result of quantum mechanics with a classical universal device.” [Bell 1964]

(Proof omitted.)

Standard modern argument

- A state of the physical system corresponds to a function assigning a value to every basis configuration.
- The number of states is thus exponential in the size of the system.
- Moreover, these values are continuous.
- Different computational paths may add up.
- Nature makes this computation efficiently.
- But can a classical computers do so?

Sure. I've just described probabilistic classical physics and probabilistic classical computation.

Quantum vs. classical

- A classical (stochastic) state is represented by probability function:

$$P(x,p)$$

- A quantum (mixed) state is represented by a "state matrix" function:

$$\rho(x,x')$$

- The state matrix behaves like probability in many ways, except it may be <u>negative</u> (or complex).

(Note that the state matrix formalism differs from state function formalism more often employed in quantum computation.)

Negative “probabilities”

- Conveniently, quantum mechanics does not allow measurement of arbitrary “events” over this “probability space” (the Uncertainty Principle).
  The allowed events have non-negative probability.
- But <u>inside</u> the computation, you can get spooky behavior with no classical analog: <u>interference</u>.

- Contradicts locality, by Bell's theorem.
- We assumed locality for the computer.
- Hence, can't simulate that classically.

(Implicitly assumes a locality-preserving mapping of the physical system to the computer.)

Can't we?

- Explicit simulation
  - Explicitly keep track of the full state matrix $\rho(x,x')$ and compute its evolution.
  - Exponential in number of the size of the system, contradicts “proportional size” requirement.
- Summation along computational paths
  - Quantum mechanics is linear
  - Do a depth-first search on the computation tree; compute the “probability” of each path separation and keep a running sum.
  - Exponential time, polynomial space   (BQP in PSPACE)
  - Essentially: path integral [Feynman 1948]
  - (No discussion of time complexity.)

A side remark:.

3. Can quantum physics be simulated by a quantum computer?

4. Can this simulation be universal?

A quantum computer

- If physics is too hard for classical computers, then build a physical computer that exploits that power.
- "It does seem to be true that all various field theories have the same *kind* of behavior, and can be simulated every way."
- Example: phenomena in field theory imitated in solid state theory (e.g, spin waves in spin pattice imitating Bose particles in field theory).
- Proposes to investigate the simulability relations between different (quantum) physical systems.
  Quantum analog of Church-Turing thesis.
- Conjecture: there exists a "universal quantum simulator" which is physically realizable and can simulate any physical system.

A universal quantum simulator

- ”I believe it's rather simple to answer that question [..], but I just haven't done it.”
- Proposes (the basis of) a solution:
  - Two-state system (e.g., polarized photon) with the 4 Pauli operators operators
    A qubit [Schumacher]
  - Many copies with local coupling
- Conjectures universality.
- (No proof or suggestion of concrete realization.)

Feynman's conclusion

“Nature isn't classical, dammit, and if you want to make a simulation of Nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.”

Quantum computation: progress

- Universal (inefficient) quantum Turing machine [Deutsch 1985]
- Universal (efficient) quantum Turing machine [Bernstein Vazirani 1993][Yao 1993]
- Equivalence between quantum Turing machines and (uniform) quantum circuits [Yao 1993]
- Quantum complexity theory [Bernstein Vazirani 1993]
- Separation results: relativized, communication complexity
- Factoring [Shor 1994]
- Promise problem [Simon 1994]
- Quantum searching [Grover 1996]
- Quantum error correction [Knill Laflamme 1996]
- Quantum cryptography (e.g., key distribution)
- Entanglement
- Experimental realizations

Quantum computation: challenges

- Practice
  - Controlling decoherence
  - Scalable implementations
  - Programming paradigms
- Theory
  - New algorithms and protocols
  - New settings (e.g., game theory)
  - Structural complexity, proving separations
  - Convincing the skeptics