Computing to Learn Physics while watching computers grow up

Gerald Guralnik*

HET — Physics Dept, Brown University, USA†.

*gerry@het.brown.edu

†www.het.brown.edu

Theoretical physicists used to think that using a computer was disgusting! Some still do. . . Many changed their minds, though.

It became clear, in the late 70's (with considerable thanks to Ken Wilson), that, in fact, computers were becoming powerful enough to solve analytically intractable (and, as it turns out, badly formulated) problems involving the most basic ideas in physics.

I mostly work in high energy theory studying problems in Quantum Field Theory (and, recently, in String Theory). While I have often been very involved in computing, I am not a "professional" and, probably, am not a "computational physicist" in the present sense.

To understand why computers work for basic (abstract) physics, define Quantum Field Theory:

- **Field Theory**: degrees of freedom at every point in spacetime. Electromagnetism is an example: $\vec{A}(\vec{x},t)$ and $A^0(\vec{x},t)$ form $A^\mu(\vec{x},t) = (A^0(\vec{x},t), \vec{A}(\vec{x},t))$ (relativistic notation); &

- **Quantum Mechanics**: equation of motion,

$$\vec{p} = m\,\frac{d\,\vec{r}}{d\,t}\;;$$
$$\frac{d\,\vec{p}}{d\,t} = 0\;.$$

Hamiltonian:

$$H = \frac{\vec{p}^{\,2}}{2\,m}\;.$$

Action:

$$S = \int \Big(p\,\dot{q} - H \Big)\, dt\;.$$

Commutation Relations ($\hbar = 1$):

$$[\,p(t), q(t)\,] = -i\;.$$

- **Quantum Field Theory**: Field Theory with Quantum Mechanics at every spacetime point! (E&M a bit complicated.)

Look at the *scalar* QFT with *one* field $\phi(\vec{x}, t) = \phi(x)$:

$$S = \int \Big(\phi^0 \, \dot{\phi} - H(\phi^0, \dot{\phi}, \text{others})\Big) \, dt \, d^3x \; .$$

The simplest form this can take to treat space and time symmetrically is:

$$S = \int \Big(\phi^\mu \, \partial_\mu \phi - \frac{1}{2} \phi^\mu \phi_\mu - \frac{m^2 \, \phi^2}{2}\Big) \, d^4x \; ;$$

$$\Rightarrow \; \phi^\mu = \partial^\mu \phi \; ,$$

and

$$(\partial^2 + m^2) \, \phi = 0 \; .$$

With (arguing in analogy):

$$i\left[\frac{d\,\phi(\vec{x},t)}{d\,t},\phi(\vec{y},t)\right]=\delta^{(3)}(\vec{x}-\vec{y})\ ,$$

One may also write,

$$S=\int\left(\frac{1}{2}\,\partial_\mu\phi\,\partial^\mu\phi-\frac{m^2}{2}\,\phi^2\right)d^4x\ .$$

A *fully equivalent* formulation was introduced by Feynman and gets rid of the operators:

$$\mathcal{Z}\equiv\int\exp\left\{\int\left(\partial_\mu\phi\,\partial^\mu\phi-m^2\,\phi^2\right)\frac{d^4x}{2}\right\}[d\phi]\,,$$

where $\mathcal{Z}$ is the **Generating Functional** in Euclidean space (a.k.a. vacuum-to-vacuum amplitude), $\partial_\mu\phi\,\partial^\mu\phi=-(\partial_0\phi)^2-\nabla\phi\cdot\nabla\phi$ and $[d\phi]=d\phi(x_1)\cdots d\phi(x_N)$. $L_0(x)=\frac{1}{2}\,[(\partial_0\phi)^2-\nabla\phi\cdot\nabla\phi+m^2\phi^2]$, positive definite, is well defined for real integration. Thus,

$$\mathcal{Z}=\int\exp\left\{-\int\,L_0(x)\,d^4x\right\}[d\phi]\,.$$

All information in a QFT can found if one knows the Green's Functions,

$$G_n(x_1, \ldots, x_n) \equiv \int \phi(x_1) \cdots \phi(x_n)\, e^{-\int L(x)\, d^4x} [d\phi] \,.$$

For $L = L_0$ one can work out this integral but, for $L(x) = L_0(x) + \frac{g}{4}\phi^4(x)\ldots$ We have a **real** problem ! For n points in each spacetime direction this involves n^4 integrals!

This is an almost *trivial* problem compared to the ones we need to solve, but it is not really well understood.

Real problems have dozens of variables at each point and, even worse, their form is not so simple. They look more like:

$$\mathcal{Z} = \int \mathrm{det}\{f(\phi)\}\, e^{-\int L(x)\, d^4x} [d\phi_1] \cdots [d\phi_n] \,.$$

It is estimated that reasonably accurate calculations could take 10, or more, tera-flop years!

Evolution of computing from my physics viewpoint:

- **Pre Monte Carlo Field Theory**:
  - Undergraduate: Course at MIT in computing (late 50's). Course started with lessons in soldering !
  - Multics: I saw a demo of the first time-sharing system in the mid 70's (Honeywell 6180 supercomputer), I dreamed of solving QFT with a machine.

    MULTICS is the mother of:

    1. UNIX: Castrated MULTICS; &
    2. VMS $\rightarrow$ Windows NT $\rightarrow \cdots$
  - Punch card solutions of differential equations on Brown's IBM mainframe;

- Cont. . .
  - Mid 70's: Macsyma on MIT, PDP 10 helped solve "non-perturbative" approximations to QFT;
  - Visited Los Alamos and dialed MIT (eventually used DARPA net): Dedicated line from my office at Brown to Boston with an extension in my home;
  - Ideas about how to do better than standard approximation techniques;
  - Late 70's: calculations on Brown's VAX 11/780's. Early 80's: used Peter LePage's VEGAS code.

- **Monte Carlo**: Seminal papers by Wilson (from the mid 60's), Creutz, Creutz Jacobs and Rebbi in the late 70's. The quest for *machine power* begins !

I started work with Don Weingarten on QCD using Brown's 11/780's with 2Mb of memory and 60Mb of disk. Peak speed less than 1 MegaFLOP !

Looked at lattices just about big enough to squeeze in the proton: $6^3 \times 14$.

A VAX was the most powerful modern machine available at a university. We had access to 3: 2 at Brown and one at Indiana. Calculations took months!

There were a handful of aging CDC 6600's in university's: 9 MegaFLOPS (introduced in 1964), designed by Sigmour Cray.

No CDC 7600's designed in 1969 by Cray — 40 MegaFLOPS.

No Cray 1's, 1976 — 160 MegaFLOPS, 1 megaword (8Mb) of memory.

Only National labs had supercomputers that might be accessible to academics. In general, computers (or terminals) were not available to theoretical physicists.

I did manage to talk DOE into (almost) giving me US$ 30K to buy a 200Mb disk for Brown's VAX.

For reasons I still do not understand, this infuriated some of the other theorists at Brown. I took the easy path and cleared out for Los Alamos in 1983.

Los Alamos was a playground of machines, mostly Cray 1's. They did not know that theorists were not supposed to do numbers, but they did know that their machines were mostly to design weapons. at that time, the director wanted to be able to claim general scientific credibility to the U.C. lab governors, so I argued my way into getting standby time on Cray systems.

This was a nightmare... But we did a lot of good physics!

I managed to interest Tony Warnock — a genius who played a Cray like a piano — and Chuck Zemach — an equally brilliant man, trained as high energy theorist and a former (full) professor at Berkeley — in the cause. With my physics knowledge and their computational and algorithmic skills, we did what was amazing!

After we got going, I managed to add some dynamic (and very difficult) young physicists to our group:

- Rajan Gupta (more energy than Saud Arabia);
- Steve Sharp;
- Aporva Patel;
- Greg Kilcup; &
- Tsutomu Shimomura (famous now for computer security — the man who jailed Mitnik).

We had an enormous amount of fun and played a dominant role in QCD computing for a year or two. Some (but not all) due to our machine access.

"How did we get cycles?"

- Prayed for machine downtime-running jobs by hand allowed us a few minutes before the batch jobs cut in;
- Loved holiday's — batch jobs ran out !
- Free loaded off of Cray research testing new machines;
- Multi-processor (4) XMP's came along with 330 megaFLOP peaks, 4 megawords (32Mb) of memory and 128Mb solid state disks;
- Supercomputer centers (non-classified) came into existence: NERSC (DOE) and Pittsburgh (NSF) were the ones we mostly used.

Good runs at NERSC in 1985 when the Cray II (2 gigaFLOPS peak — 4 CPUs — and 2Gb of main memory with a small cache) was brought on line with almost no software.

Various moderately unfruitful runs with CDC Cyber 205.

While at Los Alamos, I also tried to pick up Macsyma development using "DOE Macsyma" and leading the effort with Jim O'Dell — one of the original Macsyma developers. The Macsyma guys made the high energy theorists look docile and sane. This drove lab management nuts!

We started running into trouble every time a prediction for an underground test was wrong. Our group was blamed for "stealing" computer time. DOE called me and asked that we stop publishing computer times.

The lab also became very unhappy about the number of rental cars our bunch totaled.

All in all, I decided life was better at a university and returned to Brown in 1987.

While I remained part of our collaboration for some time, I really had enough of big collaborations (although our group was the prototype for much bigger groups which exist today).

There was a new problem: It was still hard to convince DOE to give money for local machinery. We (Kilcup and myself at Brown) had nothing to work with! Eventually, we talked DOE into buying us a couple of Sun's.

We still had the problem that we did not have any significant computing power at Brown, which we needed for serious development. DOE and NSF were, now, firmly committed to super computer centers, including the Princeton center, which McCrory, Orzag and I had started negotiating for in the early 80's.

This resulted in a long campaign by several of us, at Brown, to get funding to buy near-center quality machines for Brown. A few years ago we got NSF to fund an infrastructure grant that allowed us to build a "cave" and buy an IBM SP configuration. We are in the process of evolving this facility into an academic center.

Both, NSF and DOE, have recognized that there needs to be hierarchy of computing power and that theoretical physicists are allowed to do numbers!

However, my previous chairman was, and still is, very offended at this claim.

Theoretical Physics at Brown has 2 (aging) Cray mini-supers, a growing Linux cluster and several surprisingly fast multi CPU Sun servers.

I have got out of the, now conventional, Monte Carlo QCD business, and am thinking about alternative, more flexible, ways to compute in QFT/ String Theory.

One of the problems I am working on is studying how you can numerically calculate in the many phases that are possible in most QFT's.

The conventional Monte Carlo approach is very limited because if any term in the (Euclidean) action is not positive, the approach probably will fail.

Implicit, in our definition of path integral for numerical work is that all the integrations are on the **real** axis. If not, the positivity is effectively violated!

Returning to our early example, if we introduce a source, $J(x)$, we can define a quantity,

$$\mathcal{Z}_J = \int \exp\left\{ - \int \left[\frac{1}{2}\,\partial_\mu\phi\,\partial^\mu\phi - \frac{m^2}{2}\,\phi^2 - \frac{g}{4}\,\phi^4 + J\,\phi \right] d^4x \right\} [d\phi]\ .$$

Note: all Green's functions of the theory can be generated by (functionally) differentiating wrt J:

$$\begin{aligned} G_n &= \left\langle \Big(\phi(x_1)\cdots\phi(x_n) \Big)_+ \right\rangle \ ; \\ &= \left(\frac{\delta}{\delta\,J(x_1)} \cdots \frac{\delta}{\delta\,J(x_n)} \right) \mathcal{Z}_J \Bigg|_{J=0} \ . \end{aligned}$$

Now, let's look at a special case — **zero** dimensional QFT — only one point:

$$\mathcal{Y} \equiv \mathcal{Z}_J = \int \exp\left\{ -\frac{m^2}{2}\,x^2 - \frac{g}{4}\,x^4 + J\,x \right\} dx\ .$$

$\mathcal{Y}$ satisfies:

$$\mathcal{Y}\,\frac{d^3\,\mathcal{Y}}{d\,J^3} + m^2\,\frac{d\,\mathcal{Y}}{d\,J} = J\ ,$$

as long as the contribution to the integral vanishes at the end points. There are three independent paths that meet this condition. These correspond to the three solutions to the differential equation.

Since,

$$\mathcal{Y}[J] = a_0 + a_1\,J + a_2\,J^2 + a_3\,J^3 + \sum_{i=3}^{\infty}\,a_i\,J^i\ ,$$

we need to insert further conditions to define a_1, a_2, a_3. The only solution picked up by a real path integral sets $a_1 = 0$ and sets the Green's functions to be regular when $G \to 0$. All **odd** Green's functions vanish!

Until the 60's, the **even** solutions were the *only* ones known in QFT. The cases excluded, the **symmetry breaking** solutions, are the ones that are known to form the basis of modern explanations of particle physics (standard model).

They are really interesting solutions, because, at first glance, the conditions of **relativity** require the existence of **massless**, **spin zero**, particles (Goldstone bosons, Nambu).

However, one of the major **surprises** of QFT is that when these massless particles are coupled with gauge fields (E&M, or Yang-Mills), the theorem — for subtle reasons — no longer holds and there are no massless scalars or photons. This phenomenon (Guralnik, Hagen and Kibble — and less generally shown by Brout and Englert, Higgs and maybe Anderson) is the basis of the unified theory of weak interactions.

Two nobel prizes:

1. Salam and Weinberg (Glashow lumped in), 1979 (for the model using this effect); &

2. 't Hooft and Veltman, 1999 (for showing the theory can be made finite).

A **scalar** particle, "God particle", is predicted, which has not yet been observed.

"How do you numerically analyze this phase?"

In general, how do you directly deal with phases numerically?

With my students, I have found two possible and very promising approaches.

One is an entirely new method, applied to the functional differential equations (not the path integral) in the presence of sources. This method — **Source Galerkin** — is a `weighted residual` method and, while requiring physics (symmetry and lots of computer algebra in the setup) is (where tested) very fast, very accurate and deals with fermions (the source of the determinant) quickly and well. Variants of this method specialized to conventional perturbation theory, give impressive speed and accuracy.

The other method is a Monte Carlo approach, which is tuned around the stationary phase points of the integrand. This method is not restricted by the positivity conditions of the direct brute force approach.

Conclusion:

We have just begun to calculate!