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PART I

Watch all of the four two-video sequences titled Industrial Math Case Studies created by PIC MATH. In each of the two-video sequences, there are two videos featuring (i) a mathematical scientist discussing an industrial research problem and (ii) a faculty member discussing one possible mathematical approach that could be used to gain insights into the presented industrial research problem. After you watch all four two-video sequences, pick one of the four two-video sequences and answer the following questions: [1]

- **1.** Summarize the quantifiable question(s) being solved in the modeling effort.

  Answer. The issue at hand is the modeling of filtration systems, with the end goal of producing filters that are as effective as possible at trapping particles. Dr. Swaminathan explains how he has to use network theory to characterize the medium through which the fluid flows through (i.e., the mesh, or filter). As for the fluid itself, it is modeled via approximations to the Navier-Stokes equations. □

- **2.** In what ways did the model developed encode the causal structure of the application? Please explain. (Guiding Principle # 1: Identify the governing (physical) principles of the phenomenon seen in the application field.)

  Answer. The representation of the porous medium as a network of cylindrical capillaries seems quite accurate, and certainly more realistic than other much simpler flitration models I have seen before (e.g., the "*pancake model*"). Consequently the fluid flow couldn't be modeled via some "vanilla" ODE, and instead it requires the full machinery from the Navier-Stokes equation. □

- **3.** Did the modeler explicitly or implicitly discuss the dimensions of relevant quantities? Explain. (Guiding Principle # 2: Identify, document, and analyze the consistency of the dimensions of relevant quantities of your studied phenomenon in the application field.)

  Answer. He made no explicit mention of the units being used, but he is talking about *flow* and a *3D network system* representing the medium, so from here it is no rocket science to infer what the relevant units are. □

- **4.** Did the modeler discuss the assumptions/simplifications they made to construct the model? Did they explain how to derive a simpler or a more complex model? Explain. (Guiding Principle # 3: Construct your model with a simpler model and a more complex model in mind.)

  Answer. In order to look for the most efficient way to manufacture these filters, the modeler is attempting to create a model with as little assumptions as possible. The characterization of the porous medium on a microscopic scale as a network of cylindrical capillaries, and the simulation (via Navier-Stokes) of particle flow and capture assuming a rather elaborate geometry, make the final model quite robust (at least it does seem that way to a non-expert like myself). He did not make mention of a possible simpler model, although he does go on to say that the alternative to the modeling would be a bute-force construction of the filters' design, which would entail a trial-and-error approach (and this is obviously not something that the company would be happy about!). For what is worth, we did discuss some simpler filtration models in Math 622. . . □

- **5.** Explain how the application motivated the model. Was there any evidence of the modeler continual integrating the application, the mathematical model, and the math analysis/computations? Explain. (Guiding Principle # 4: Exhaustively integrate the application field, the process of mathematical modeling, and the mathematical analysis/computations.)

  Answer. The purpose of any filter is to trap particles, while not interfering with the fluid flow. To that end, a good model must consist of both a good (abstract, mathematical) candidate for the filtering material, and realistic governing equations of the fluid flowing through this material. The former motivates the choice of the network model over something simpler but less effective such as, say, a two-dimensional sheet-like membrane with holes in the surface. Consequently, the use of this more complicated geometry to simulate the material requires a more thorough mathematical treatment to describe the dynamics of the fluid going through; this is where the Navier-Stokes equations come into the picture. □

[1] I chose the ***Building a Better Filter*** two-video sequence.

- **6.** Did the modeler discuss how they did or could verify and validate the model? Explain. (Guiding Principle # 5: Verify and validate your model by comparison with data.)

  Answer. He did mention that after the simulation one should see where the (virtual) particles fell in the simulation network, and compare those results to a real-life counterpart experiment where particles are being streamed through the filtering material. □

- **7.** If you were building off the modeling efforts discussed, what would you do next? Explain.

  Answer. Perhaps use machine learning to somehow create even more intricate networks that optimize the particle-trapping? □

PART II

In the second part of the assignment, you will reflect on the modeling you did for your final project in MATH 622.

- **1.** Write a one-page succinct summary (300-500 words) of your model developed last semester. (Note that you will be asked to do this on the math modeling qualification exam.)

  Answer. In the project I presented a study of bubble nucleation in phase transitions of the early universe, modeled via a theoretical scalar field known as an *instanton* (or *caloron*, in the thermal case). Such field posseses a multi-minima potential; one such minimum being a false vacuum (local minimum) and the other one being the true, absolute vacuum state (global minimum). I investigated both the zero-temperature (instanton) and finite-temperature (caloron) cases, where we see how the effects of quantum tunneling and thermal fluctuations enter the picture of the false vacuum decay. I presented results in up to three spatial dimensions, ignoring gravitational effects and assuming rotational symmetry of the bubbles in the spatial dimensions.

  In semi-classical studies of the false vacuum decay, one considers the decay rate of an instanton, i.e., of a field solution to the imaginary-time classical equations of motion. Such solutions are subject to a quantum effect known as *barrier penetration* (or *quantum tunneling*), which is forbidden at the classical level but are very much present in the quantum realm. It turns out that the nucleation and decay of such scalar field solutions may just have played a significant role during first-order phase transitions in the early universe; thus analyzing the transition from vacuum decay to thermal decay of these instantons is of great importance. Such transitions are associated with supercooled states and the nucleation of bubbles. They arise in a wide range of applications, from the condensation of water vapor to the vacuum decay of fundamental quantum fields. In cosmology, bubbles of a new matter phase would produce huge density variations, and (unsurprisingly) first-order phase transitions have been proposed as sources of gravitational waves and of primordial black holes. In a cosmological context, the temperature is falling as the universe expands, and at some stage the rate for the first-order phase transition becomes smaller than the rate of vacuum decay.

  In the project I presented new numerical methods (co-developed by myself and my previous supervisor from Newcastle University, Ian G. Moss), which allow the vacuum-thermal crossover to be studied in detail for the first time, since traditional shooting methods break down in the thermal case due to the lack of rotational symmetry of the bubble. Thus, the project entailed both a *computational physics* problem and a *modeling* problem. The former is showcased via the aforementioned novel computational technique that successfully tackles both the instanton and caloron decays, while the modeling component shows both the effect of temperature on vacuum decay and bubble formation and also a (quite mysterious!) link between the height of the potential barrier of the scalar field used in the model and the action of the field. The more surprising bit is not that there is a correlation between these parameters, but rather that this relation is (very!) linear. Previous work on this topic (see my paper) has revealed this strange relation in the 1+1D case. In the Math Modeling I project I showed that this linear fit (remarkably) still holds quite well in up to three spatial dimensions. □

- **2.** Next, answer the following questions:

  - **a)** Summarize the quantifiable question(s) you answered in your MATH 622 final project.

Answer. I found out that as we increase spatial dimensions, the transition from vacuum to thermal state takes place earlier (meaning, at lower temperatures). Furthermore, I found a surprisingly linear relation between the action of the field and a parameter that is related to the height of the potential barrier (i.e., the barrier between the local and global minima). This parameter appears in the potential, and the potential itself contributes to the total Euclidean field action, so it is not shocking to see a relation between the aforementioned parameter and the action. The surprising bit is that this relation is very linear, which is not obvious at all. The possible physical implications of this linear correlation between the height of the barrier and the total action is not yet well understood. □

– **b)** In what ways did the model you developed for your MATH 622 final project encode the causal structure of the application considered? Please explain. (Guiding Principle # 1: Identify the governing (physical) principles of the phenomenon seen in the application field.)

Answer. The model tackles a well-known problem in early-universe cosmology, and it is founded on earlier work that proposes that bubble nucleation can be studied in a laboratory cold-atom analogue of cosmological vacuum decay. While, traditionally, analogue systems have mostly been employed to test ideas in perturbative quantum field theory, there has been recent interest in using such analogue "table-top" experiments on nonperturbative phenomena such as bubble nucleation. Through "modelling the universe in the lab" we hope to gain a better understanding of the process of vacuum decay and the role of the instanton. This is particularly relevant nowadays in light of the recent measurements of the Higgs mass, which currently indicate that our universe's vacuum is in a region of *metastability*. The model presented in Math Modeling I is an extension of earlier numerical attempts that relied on shooting methods, which were only effective when the rotational symmetry of the bubbles is also assumed in the imaginary-time dimension (thereby excluding thermal effects). This new computational technique, on the other hand, successfully tackles both the instanton and caloron models. □

– **c)** In what ways, did you use dimensions to help you with your model development for your MATH 622 final project? Explain. (Guiding Principle # 2: Identify, document, and analyze the consistency of the dimensions of relevant quantities of your studied phenomenon in the application field.)

Answer. In no way whatsoever. It is common practice in certain applications of theoretical physics to use "natural units" (aka "geometrized units" or "Planck units"), where all relevant physical constants (e.g. the speed of light, Newton's constant of gravitation, the Planck constant, etc) are set equal to 1 (a succint one-page explanation of this convention can be found on my Github). Nevertheless, the translation of the relevant quantities in my model to physical units is explained in the Conclusions of my paper. □

– **d)** What were the key assumptions/simplifications you made in the construction your model? Is there a simpler model you could derive? Is there a more complex model you could derive? Explain. (Guiding Principle # 3: Construct your model with a simpler model and a more complex model in mind.)

Answer. The key simplifications in my model were the imposition of rotational symmetry in the spatial dimensions and the lack of gravitational effects. In this picture, the behavior of the scalar field is modeled as a second-order, damped-oscillator equation in relaxation time

$$\boxed{\frac{d^2\Phi}{ds^2} + k\frac{d\Phi}{ds} = \Delta^\dagger \mathscr{F}} \tag{1}$$

Here k is a damping coefficient, s is the relaxation time, Φ is an (auxiliary) scalar field (which approaches the bubble solution Φ_b as $s \to \infty$), $\mathscr{F}$ is the error residual, and $\Delta^\dagger$ is a second-order differential operator. I did attempt two simpler versions that also satisfy the equations of motion of the scalar field, but neither attempt was successful. The simplest case is given by

$$\frac{d\Phi}{ds} = \mathscr{F}. \tag{2}$$

In this equation, as $s \to \infty$ the residual goes to zero, meaning that the scalar field relaxes to a steady-state. The problem here was numerical instability. A perturbation $\delta\Phi$ on the auxiliary field then revealed that the behavior of the system close to the bubble solution Φ_b is governed by a second-order operator. Thus an improvement of (2) is

$$\frac{d\Phi}{ds} = \Delta^\dagger \mathscr{F}. \tag{3}$$

This particular equation does work, but upon performing a von Neumann stability analysis, it is revealed that this choice requires a very small numerical relaxation time step ($\Delta s \sim O(\mathrm{h}^4)$), so it is rather impractical. A similar stability analysis on Eq. (1), on the other hand, shows that this algorithm only requires $\Delta s \sim O(\mathrm{h}^2)$, which is much more practical. As to whether there could be a more complex model I could build to tackle this problem, the answer is: **absolutely!** . . . I will elaborate more on this on part g), but let's just say for now that gravity has not entered the picture at all in all this work. □

– **e)** Explain how the application motivated the model developed for your final project. Give an example of how you integrated the application, the mathematical model, and the math analysis/computations in your final project modeling effort. (Guiding Principle # 4: Exhaustively integrate the application field, the process of mathematical modeling, and the mathematical analysis/computations.)

Answer. The motivation comes from recent measurements of the Higgs mass, which indicate that the Higgs potential develops a lower energy state than the electroweak vacuum. Consequently, the quantum phenomenon known as *barrier penetration* (aka *quantum tunneling*) might lead to a disastrous decay of our universe's vacuum. (However, one may be relieved to know that, at least according to the currently established Standard Model parameters, our vacuum's lifetime seems to greatly exceed the present age of the Universe. Therefore our vacuum is in a region of *metastability*; it is in a *false vacuum state*.) The integration of this issue of the vacuum decay with the instanton picture is not even remotely an original idea of mine (if only!), but rather it was put forward in the 1970's by Sidney Coleman in an effort to tackle the vacuum decay problem using semiclassical techniques (meaning, not only approach it from a quantum physics point of view, but also using a field theoretical approach). Since then there has been several succesful numerical methods (mostly using shooting methods) to tackle the problem, [2] but very little progress when thermal fluctuations are taken into consideration. This is where my newly-developed algortithm comes into play. □

– **f)** Did you verify/validate the model you developed last semester? If so, how? If not, how could you? (Guiding Principle # 5: Verify and validate your model by comparison with data.)

Answer. The model was tested extensively, both for numerical accuracy and for the validity of the underlying theory. However, an instanton is a theoretical particle, and the whole model is based on it, so a hands-on real-world lab testing is not so straightforward. There are indeed analogue ways to test phase transitions and vacuum decay using *Bose-Einstein condensates* in an actual lab, but I do my part on the theory end and defer to the more practical folks for testing... (This is a gentler way of saying that I'm fairly useless). □

– **g)** If you were building off your modeling efforts from last semester, what would you do next? Explain.

Answer. Incorporate gravity in the model. To do so we must have an energy-momentum tensor field $T^{\phi}_{\mu\nu}$ for the scalar field ϕ that couples to the curvature of spacetime via the *Einstein Field Equations*

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi T^{\phi}_{\mu\nu}. \tag{4}$$

The scalar field must satisfy these (ten) equations, and must also satisfy its intrinsic equation of motion (EoM). If the scalar field is real, this EoM is the well-known *Klein-Gordon* equation

$$\nabla^2\phi - m^2\phi = 0,$$

whereas in the case of the instanton (our case), the EoM is given by

$$\mathring{\nabla}^2\phi - \partial_\phi U = 0.$$

Here U is the multi-minima potential mentioned earlier, and the $\mathring{\nabla}$ notation indicates that the time-component of the gradient is imaginary-time, as opposed to real coordinate time as in Klein-Gordon. At this point it becomes clear that we have a (big) problem: the instanton picture uses imaginary-time, while the LHS of (4) shows quantities that have only real coordinate time. (This is yet another prrof that quantum physics and gravitation don't get along too well ☹) Hence, if I continue down this route I will end up in some quantum gravity formulation, which is way outside of expertise ... Two (feasible) options remain: either I'm happy with ignoring gravity and just say the classical "meh ... gravity is too weak at such small scales anyway" (this is the solution preferred by 99.99999 % of quantum physicists), or I follow a completely different path, which has been suggested recently by Jonathan Braden. In this paper, Dr. Braden proposes an alternative picture of vacuum decay, in which the classical evolution (as opposed to the instanton's imaginary-time evolution) of the field from some initial realization of the false vacuum fluctuations leads to the emergence of bubbles. This method, however, has not yet been extended to the thermal decay. The relaxation technique I presented on my modeling project does apply to the thermal case, although the price to pay is the aforementioned miscommunication between the instanton picture and gravity. A model that successfully tackles thermal decay in the classical scene would be a nice extension to the work presented both in Dr. Braden's paper and on my modeling project. □

[2] Analytically, the problem can only be solved under some very restrictive assumptions, such as the well-known "*thin-wall approximation*" (see Coleman's paper for reference).