My two-cents experience in doing reactor physics

Yung-An Chao
November 2018 in Shanghai China

Professor Akio Yamamoto asked me if I could write an article for the Reactor Physics Division of AESJ on my experience of doing reactor physics, mainly for the interest of students and young colleagues. As I started to write it, I realized that I committed to a very challenging task when I accepted his invitation. I decided to choose a few examples to convey my way of learning and doing reactor physics. As the targeted readers are mainly students, I must apologize to more senior colleagues if the writing sounds trivial or too much preaching.

1. Two examples in text book reading:

First a very simple example. Resonance shielding is an important subject in reactor physics. To explain why a sharply peaked absorption resonance will be less absorptive than a flatter and broader resonance, text books typically show mathematically how a dipped flux spectrum results in less absorption via the evaluation of the reaction rate integral. I find it simpler to understand the physics by thinking of using a roll of toilet paper to wipe out spilled water. It is obvious that pulling out the paper from the roll will be much more effective than applying the roll directly. The outside of the roll "shields" the interior of the roll. The same analogy applies to the spatial shielding effect of a lumped fuel rod embedded in moderator versus a dispersed mixture of fuel with the moderator.

Then a little more intriguing example. The core system eigenvalue (k) and the corresponding reactivity are fundamental concepts in reactor physics. Text books tell us that a steadily operating core is at criticality, k=1. But a core cannot start by itself without some initial "extraneous" neutron source (S). A simple point model for neutron balance gives that the neutron flux level is proportional to S/(1-k), with k being the ratio of neutron production to absorption. Then how can the flux for a critical core be maintained if the flux would become infinity at criticality? The explanation is that when the core is brought close to criticality, the flux level increases rapidly to the targeted level while the core still staying just a tiny bit subcritical, never really reaching criticality. Text books always present an eigenvalue problem without including the S term in the equations, because when close to criticality S is completely negligible compared to the chain reaction neutrons and its presence has nil effect on the flux distribution. This simple point model also points to a few interesting things.

- A core steady state can occur only when it is sub-critical. When the core goes critical or super critical, it must be in a transient state. Otherwise the flux would become negative.
- If one writes a code to solve the diffusion equation in presence of S, one would run into trouble if the core is very close to criticality. To avoid this problem, one could estimate the eigenvalue on flight and switch to the eigenvalue problem when the S term becomes negligible.
- Although the flux distribution near criticality is given by the fundamental mode independent of the shape of S, in a deeply subcritical core the flux distribution may be largely affected by the S distribution. The deviation of the flux distribution from the fundamental mode distribution indicates the degree of subcriticality.
- Consequently, the effective neutron multiplicative capability of a subcritical core may be quite different from what the core eigenvalue would suggest. However, one should not be misled that one might "gain" any reactivity safety margin because of this. The safety

margin is dictated by how far the core is from criticality, which is independent of S and depends solely on the eigenvalue.

2. On nodal methods:

Nodal method has been a dominating tool in core analysis over the past thirty plus years, and likely to remain so for at least some years to come. Although I worked on it and used it myself, I have always had some reservation about it. The most popular nodal method is the transverse integration nodal method because of its simplicity and efficiency. The two pillars of the method are the discontinuity factor and the transverse leakage profile, the former of which is semi-empirical while the latter is quite ad hoc. Particularly the construction of the transverse leakage profile is quite arbitrary, as theoretically there is even no reason why the profile should be continuous across the intersect of the four adjacent nodes. The assumption for the justification is that the transverse leakage is supposed to be small, thus the result will not be so sensitive to its detailed profile. This may be adequate for diffusion calculation. But when using SP_3, as to be discussed in the following section 5, the correct interface and boundary conditions will contain higher order tangential derivatives, which is the transverse leakage on the surface. In such a case if one would still use the ad hoc transverse leakage profile, one would run into iteration instability and nonconvergence. A more rigorous solution method must be used instead. As for the discontinuity factor, it typically comes from reflective unit assembly homogenization, which is the weakest model and the biggest problem in today's core analysis method, and I believe it will eventually be the killer of today's method.

Another tool typically used together with nodal method is CMFD (coarse mesh finite difference). The classical finite difference current between two adjacent nodes is proportional to the flux difference $\phi_L - \phi_R$. CMFD makes a simple revision to it by adding another term proportional to the sum $\phi_L + \phi_R$. The coefficient of the difference term is theoretically well known, while the coefficient of the sum term is empirically determined by brute force matching the CMFD neutron current to the current from the higher level nodal method calculation. Although with no theoretical justification, this recipe works because of having one additional free parameter to play with. I did not feel comfortable about it and hesitated to use it until I could understand it. I noticed that this recipe simply means a general linear combination of the two fluxes, i.e. $D_L\phi_L - D_R\phi_R$, and this form can be rigorously derived in the 1D case with both D_L and D_R analytically determined. The argument goes as follows. In 1D case, the analytic flux solution in each of the two adjacent nodes has two free parameters. The four free parameters in total for the two nodes are reduced to two by imposing the flux and current continuity condition on the interface. Hence there is only one free parameter per node, which can be chosen as the node average flux. Therefore, it must be possible to analytically express the interface current in terms of the two fluxes only. Pursuing along this line I derived the Analytic CMFD (ACMFD) equations for the diffusion case in both Cartesian and hexagonal geometry. (I also derived the ACMFD coefficients for the transport case, although I never had a chance to implement it.)

A popular use of CMFD in nodal method is the so called two nodes model, where the higher level nodal calculation is done only for two adjacent nodes to determine the CMFD coefficients. The full core calculation is then done only with CMFD, which in turn provides the boundary value of the two nodes problem. Personally, I think relying only on the (empirical) CMFD for the whole core calculation is risky and I have a concern that the iteration may not be robust for all engineering problems. I prefer to use CMFD/ACMFD purely as an acceleration tool such that thru the iteration process both the lower level CMFD and the higher level nodal method calculation are done for the whole core problem. In

case the acceleration piece would cause any problem, the design code could automatically turn it off to assure convergence.

3. On conformal mapping:

By late 1980's the transverse integration nodal method had become the mainstream solver because of its simplicity and efficiency in engineering applications. When people tried to apply the method to hexagonal geometry, they ran into the difficulty of how to handle the resulting severe singularity at the vertices of the hexagon. This problem caught my interest. I recalled what I read in my school days that in classical electrostatics people used in early days conformal mapping to do the design of electric capacitor of different shapes because the Laplacian operator ∇^2 in the electrostatic equations is invariant under conformal mapping. Since diffusion equation has the same operator, we should be able to use conformal mapping to map a hexagon to a rectangle to then apply the transverse integration method. This should alleviate the singularity problem.

Since I did not expect to have the opportunity to work on this "academic" problem in our company, I wrote a Letter to the Editor of Nuclear Science and Engineering to publicize this idea, hoping that someone would pick it up. But nobody did, and I realized that I had to do more to save this idea. I went to the company library to find a 1952 book "Dictionary of Conformal Representation" and borrowed from a colleague a floppy disc of Fortran II to work out at my home the numerical calculation of the mapping function. To be practical for implementation, the next step was to approximate the numerical results with analytic functions in a closed form. At this point a manager told my boss not to allow me wasting my time on academic work. Then an opportunity came just in time for me to make the work into a university cooperation project. To figure out the approximation function, I used what I learned in school about complex variable function that the only function being analytic everywhere (including at infinity) is a constant function. All other functions must have singularities. Thus, a very powerful and efficient way of approximating a function is to locate and best approximate its singularities.

Then the East European countries opened, and the company got interested in the refueling business of VVER reactors. Using the conformal mapping method, we could much more easily adapt the existing core design codes to hexagonal cores. Interestingly the manager who did not like me wasting time on academic work was then appointed a manager in the VVER project, and I believe he then much appreciated the value of what I persisted on.

4. On Stiffness Confinement Method (SCM) in space-time kinetics:

Stiffness in kinetics is caused by the prompt neutron lifetime being orders of magnitude shorter than the delayed neutron lifetime such that the time discretization has to take very small time steps controlled by the prompt neutron lifetime. The idea of SCM was inspired by the observation that the stiffness effect results in a prompt jump rise of the prompt neutron population while does not lead to any irregular behavior in the precursor response. This is because the precursor population is much larger while its population change is much smaller compared to the prompt neutron. By introducing a dynamic frequency, the stiffness can be effectively confined only to the prompt neutron equation which can be analytically solved after the stiffness absent precursor equation is solved. The idea was first demonstrated and confirmed numerically with point kinetics.

When generalized to space time kinetics, the dynamic frequency is split into a shape term plus an amplitude term. The shape frequency is a function of both space and time, while the amplitude frequency is a function of time only. The former is obtained from the prompt neutron shape change while the latter from the prompt neutron total population change. The prompt neutron kinetic equation is converted to an equivalent static eigenvalue equation, where the dynamic frequencies divided by neutron velocity are treated as artificial macroscopic cross-sections. If the eigenvalue is not equal to unity, then an adjustment on the amplitude frequency is made, according to the resulting point kinetic equation. This process is done iteratively until convergence. The flux distribution is then updated in both shape and amplitude using the corresponding dynamic frequencies. This method allows the use of much larger time discretization steps while still giving accurate results. But unlike other methods, when using SCM one needs to be cautious about using small time steps, which may cause instability. The convergence criteria in the SCM eigenvalue problem calculation must be compatible with the actual change of the eigenvalue and eigen function between the two ends of the time step. If the convergence residual is not negligible compared to the actual change in the time step, then the time step should be enlarged.

The above work was related to thesis research of my students. At the time our company did not find any market incentive to convert the 3D kinetics code into a commercial product, because safety analysis based on 3D kinetics was considered unnecessary. The code was put on shelf several years without transient thermo-hydraulics added to it. It was unplanned and totally unexpected that its first engineering application turned out to be the simulation of DRWM (see next section), where no thermo-hydraulics feedback is needed because the low power physics test is essentially done at zero power. Sometimes one does not know what a research project would eventually lead to.

5. On Dynamic Rod Worth Measurement (DRWM):

The problem of DRWM development is how to use a point-model based reactivity meter to analyze data from a 3D transient process. The key is of course how to account for the spatial effects. A quick physics analysis concludes that there are two spatial effects, the static spatial effect and the dynamic spatial effect. Consider a “Gedanken” experiment on a symmetric core with one control rod completely inserted and its symmetric partner completely withdrawn. If we swap the positions of the two identical rods, there should be no reactivity change of the core, yet the excore reactivity meter will record flux change and indicate positive or negative reactivity change pending on where the meter is located. This is a static spatial effect, due to core configuration change per se. The dynamic spatial effect arises because the delayed neutron distribution change trails behind that of prompt neutron. Simulation calculation can predetermine the proper signal correction factors due to these two effects. But then there is the subtle question whether the use of these correction factors would “mask” the measurement data such that the measurement result would always agree better with the core design prediction. A qualitative physics analysis shows that this correlation is generally negative, which tends to enlarge the discrepancy between the prediction and measurement. This anti-masking feature will give more conservative results, which is acceptable from the safety point of view. A large amount of simulation calculation was done to confirm the conclusion of this qualitative analysis.

When we got the first DRWM testing data from a core startup physics measurement, the discrepancy between the design prediction and measurement of rod worth was excessively large. The management decided to abandon the development project. But I noticed that the problem came from the heavy rods, one set of which was unusually heavy with 1800pcm rod worth. A simple point kinetics model indicates that the rod worth would be roughly proportional to the logarithm of the ratio of the

initial flux to the final flux. When such heavy rods were inserted the signal dropped so low that the background could severely contaminate the final flux value and thus affect the results significantly. Since the background signal should be the same for all the sets of rods, I best estimated a constant background to subtract from all the signals. All the discrepancy largely disappeared! The estimated background was a fraction of the lowest signal, which was quite reasonable. The project survived, and the background compensation has since been a crucial part of DRWM.

6. On the Generalized SP_N theory (GSP_N):

Despite its simplicity and practical usefulness, I was always a little skeptical about SP_N because of its lack of a theoretical foundation. Although I never used SP_3 myself I started to think about it more seriously when my student needed to calculate the SP_3 discontinuity factor for cell homogenization. To properly define the discontinuity factor, one needs to compare the reference transport solution to the SP_3 solution. But there is no way of deducing the reference value of the SP_3 functions from the transport solution because we don't know how to relate the SP_3 functions to the transport angular flux, thus popping up the question "what is the angular flux representation corresponding to the SP_3 solution?"

As I started to investigate this problem, I soon realized that the rigorous derivation of the SP_N differential equations for a homogeneous medium has never been a problem, which has been done in various ways by people. (To my big surprise, I discovered that the first derivation was as early as 1944 by Mark and a little later by Davison when they developed the P_N theory, although not calling it by SP_N at the time.) The problem has always been not knowing how to derive the interface and boundary conditions (IBC). In practice people have been using the (ad hoc) 1D type IBC on the surface value and the normal direction derivative of the SP_N solution functions. I then questioned why we can easily derive the IBC for P_N but not for SP_N? Physically the IBC should follow from the continuity requirement on the angular flux. In case of P_N the angular flux is represented via spherical harmonics expansion with the P_N functions as the expansion coefficients. In such a case, angular flux continuity is the same as the continuity of the P_N functions. The derivation of IBC for P_N therefore does not need the reconstruction of the P_N angular flux. For SP_N, however, there is no such a simple expansion. Therefore, in search for the SP_N IBC we must go beyond the domain of the SP_N functions to ask what is the SP_N angular flux representation corresponding to the SP_N solution functions? I faced the same question again: we don't understand the physical meaning of SP_N unless we know its corresponding angular flux representation.

I struggled with the quest for the SP_N angular flux representation for a couple of years and it eventually leaded me to the development of the GSP_N theory, where I had to learn and use the mathematical tools of solid harmonics, the Helmholtz decomposition of vector, the Davison lemma for solid harmonics, and the generalized Helmholtz decomposition of tensor. (Ironically all these tools were used or developed by Davison sixty years ago in his fascinating work of partially successful attempt to solve the P_N equations analytically.) The GSP_N theory transforms and recasts the P_N equations into N+1 layers, where each layer contains a set of diffusion type differential equations. The equations in each layer is decoupled from the other layers. Each layer contributes a piece of the angular flux which is explicitly given in terms of the spatial gradients of the layer's solution functions. The complete P_N angular flux is the sum of all the pieces contributed by the different layers. Each time when a layer is added, the summed angular flux changes such that the derived IBC changes as well. Therefore, although the diffusion type differential equations in different layers are decoupled, the IBC for the layers are nevertheless coupled depending on how many collected layers one wants to use.

The lowest layer in GSP_N is identical to the traditional SP_N except for a different IBC, which is no longer 1D type and contains higher order tangential derivatives in addition to normal derivatives. Since conventional numerical methods have difficulty of handling the higher order tangential derivatives in IBC, a new numerical method is developed to solve the GSP_N equations.

Concluding remarks:

Usually the first thing I do when I start to work on a problem is to think about the physics behind so that I can properly define the problem from the physics point of view. The crucial step is then to build a corresponding physics model, where necessary assumptions (i.e. approximations) are introduced. Henceforth it can be converted to a mathematical problem, where I may have to find or learn new mathematical tools to solve it. I am not good at reading a lot of equations, where often I quickly get lost. If I could first understand what the physics problem is, then I could more patiently focus on reading the equations repeatedly to understand it. If I cannot understand something in my own way, I have reservation on believing and accepting it.

A professor I most respected in graduate school told us “Physics is a science of approximation, and mathematics is a science of exactness. Mathematics is not physics.” When we solve a physics problem, we always need to build a model with assumptions. Building the model is doing physics, the science of approximation. But following what my professor said, I would like to add “Science of approximation does not mean approximate science.” Good physics should avoid ad hoc approximations.

Everyone has his/her own way of working and his/her own taste of appreciation. Undoubtedly my experience is very subjective and may not even worth two cents to you. But anyway, I have fulfilled my commitment to Prof. Yamamoto.

References:

CMFD/ACMFD:

- Y. A. Chao, "A Theoretical Analysis of the Coarse Mesh Finite Difference Representation in Advanced Nodal Methods", The Proceedings of M&C'99-Madrid, Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications, Vol. 1, pp.117 - 126, Madrid, Spain, September 27-30, 1999.
- Y. A. Chao, "Coarse Mesh Finite Difference Methods and Applications", Proceedings of the PHYSOR 2000 ANS International Topical Meeting on Advances in Reactor Physics and Mathematics and Computation into the Next Millennium (on CD), Pittsburgh, USA, May 7-12, 2000

Conformal mapping:

- Y. A. Chao, "Comments on the Treatment of Transverse Leakage in Advanced Nodal Codes for Hexagonal Nodes," Letter to Editor, Nucl. Sci. Eng., 1991, 109, p.423.
- Y. A. Chao and N. Tsoulfanidis, “Conformal Mapping and Hexagonal Nodal Methods – I: Mathematical Foundation”, Nucl. Sci. Eng., 1995, 121, pp.202-209.
- Y. A. Chao and Y. A. Shatilla, “Conformal Mapping and Hexagonal Nodal Methods – II: Implementation in the ANC-H Code”, Nucl. Sci. Eng., 1995, 121, pp.210-225.

Stiffness confinement method:

- Y. A. Chao and A. Attard, “A Resolution of the Stiffness Problem of Reactor Kinetics”, Nucl. Sci. Eng., 1985, 90, pp.40-46.
- Y. A. Chao and P. Huang, “Theory and Performance of the Fast-Running Multidimensional Pressurized Water Reactor Kinetics Code, SPNOVA-K”, Nucl. Sci. Eng., 1989, 103, pp.415-419.

DRWM:

- Y. A. Chao, D. M. Chapman, D. J. Hill and L. R. Grobmyer, “Dynamic Rod Worth Measurement”, Nucl. Tech., 2000, 132, pp.403-412.

GSP_N theory:

- Y. A. Chao, “A new and rigorous SP_N theory for piecewise homogeneous regions”, Annals of Nuclear Energy, 2016, 96, pp.112-125.
- Y. A. Chao, “A new and rigorous SP_N theory – Part II: Generalization to GSPN”, Annals of Nuclear Energy, 2017, 110, pp.1176-1196.
- Y. A. Chao, “A new and rigorous SP_N theory – Part III: A succinct summary of the GSPN theory, the P_3 equivalent $\mathrm{GSP}_3^{(3)}$ and implementation issues”, Annals of Nuclear Energy, 2018, 119, pp.310-321.
- Y. A. Chao, L. Peng and C. Tang, “A new and rigorous SP_N theory - Part IV: Numerical testing of $\mathrm{GSP}_3^{(0)}$ using the plane wave expansion method”, in preparation for submittal to Annals of Nuclear Energy.