NE 255, Fa16
Solution Context and Tools
September 20, 2016

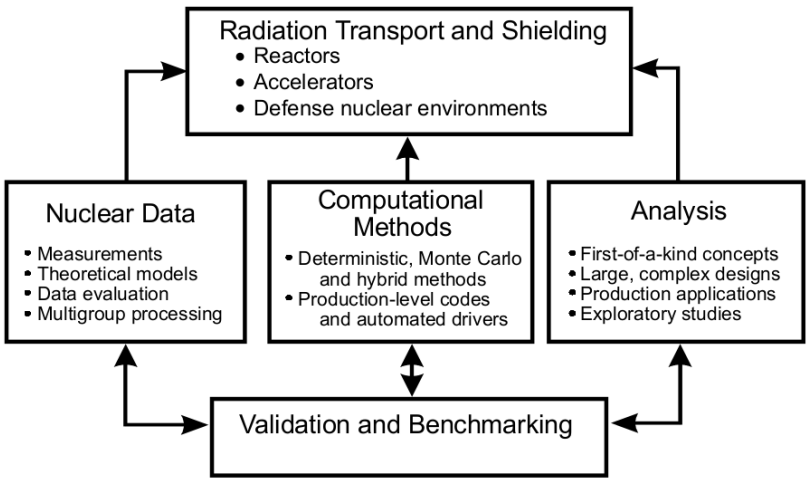
We've started looking a little bit at how to play around with the transport equation. To venture much farther in thinking about solving the transport equation, it helps to remember what we're applying it to, how we might attack actually solving it, and some other bits of information that we use.

As mentioned, we'll mostly focus on reactors in this class. A nuclear reactor is a three-dimensional structure consisting of complicated geometrical shapes made of variety of materials.

- A unit cell usually consists of a fuel rod, gap, cladding and corresponding moderator. It is usually surrounded by similar cells. A fuel rod consists of fuel pellets.
- A fuel assembly usually consists of several hundred fuel rods (fuel cells).
- A reactor core consists of several hundred fuel assemblies.
- Fuel assemblies and fuel rods are usually arranged in square or hexagonal lattice.
- Instead of fuel pellets, the fuel could be in the form of coated fuel particles (TRISO particles).
- Coated fuel particles could be arranged into fuel compacts or pebbles (Pebble Bed Reactor).

(switch to ppt for image examples)

Solution Context and Data



We have many different types of geometries and physics going on with the systems we're interested in. However, we take the same fundamental approach no matter what. Each component is

incredibly important, but let's take a moment to talk about **Nuclear Data**.

We need a description of all of the physical interactions happening inside a nuclear reactor that we can use in our equation. An *evaluated nuclear data file* is a collection of various data enabling to reconstruct, for each isotope, its cross-section's

- general information
- resonance parameters
- angular distribution for emitted particles
- energy distribution for emitted particles
- energy-angle distribution for emitted particles
- thermal neutron scattering law data
- radioactivity and fission-product yield data
- multiplicities for radioactive nuclide production
- cross-sections for radioactive nuclide production

There are many evaluations coming from various countries such as: USA, Europe, Japan, Russia, China, ... Getting from experimental data (what we have of it) + theory (however accurate that is) to data that can actually be used in a code is no small feat. And, that process is sort of a mess...

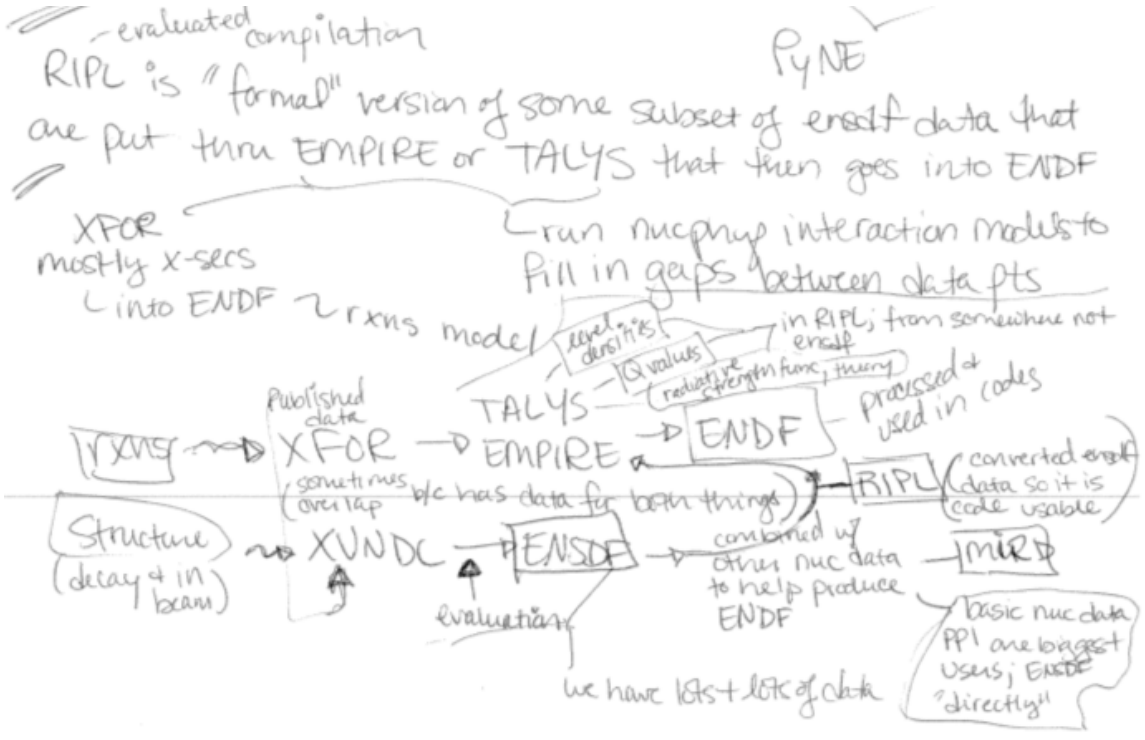


Figure 1: Notes from a meeting where someone tried to explain this to me

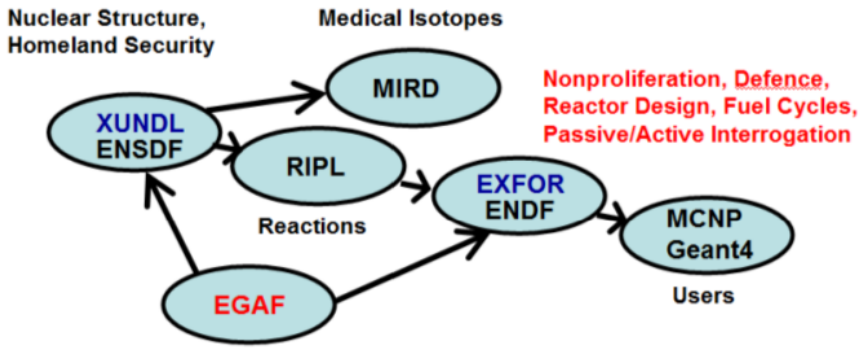


Figure 2: A more coherent (but less comprehensive) set

We won't go through all of this, but I think it's important to have context about what this is and how confusing it can be. There is a lot of data and many formats. In computation you will pretty much only need to interface with ENDF and its equivalents.

The data that we use is complicated, and can be quite different depending on the application we're interested in. Let's look at some (back to ppt).

Physics Impacts

We are often able to use knowledge about the physics to inform method development or, at the very least, choose which methods are more appropriate given our physics.

For example, you may notice is how, in particular, Fast and Thermal reactor physics differ. We often need different codes to deal with LWRs and FRs (note: CASL and NEAMS are different initiatives...). Many of the assumptions employed in traditional LWR methods do not apply:

- Lack of a 1/E energy spectrum as a basis for the calculation of resonance absorption.
- Upscattering resulting from the thermal motion of the scattering nuclei may be neglected.
- Inelastic, (n, 2n), and anisotropic scattering are quite important.
- Long mean free paths imply global coupling. That is, local reactivity effects impact the entire core.
- The energy range where neutrons induce fission and the energy range where the fission neutrons appear strongly overlap.

Other physics considerations have high priority in FR methods

- Detailed energy modeling for resonance structure (core/reflector).
- Transport and anisotropy effects are more important at high energy.

In general, a distinct set of physics analysis and core design tools with tailer assumptions have been and are being developed for FR analysis.

Computational Methods

Inside the box of computational methods, we have two main categories:

- **Deterministic**: discretize all independent variables, obtain a set of coupled, linear, algebraic equations and develop a numerical method to solve them.
- **Probabilistic**: follow the history of each relevant particle based on the underlying probabilities for various types of interactions.

Everything we've done so far applies to both methods (we haven't discretized, only simplified). Each method has its own benefits and challenges. We'll talk a bit about **deterministic first**. Here, the discretization methods are a big part of the strategy, followed by parallelization.

The size of the problems (which impacts memory and parallelization performance) is government by discretization. To get more accurate fluxes, typical transport problems today are three-dimensional, have up to thousands $\times$ thousands $\times$ thousands of mesh points, use up to $\sim$150 energy groups, include accurate expansions of scattering terms, and are solved over many directions. E.g. In 2012, a Pressurized Water Reactor (PWR)-900 with 44 groups, a 578 $\times$ 578 $\times$

Table 1: Meaning and Range of Indices Used in Transport Discretization

Variable	Symbol	First	Last	Low	High
Energy	g	1	G	2	100s
Solid Angle	a	1	n	S_2	S_{16}
Space	suppressed	n/a	n/a	1?	1e9
Legendre moment (P_N)	l	0	N	0	9

700 mesh, using S_{16} level-symmetric quadrature, and with P_0 scattering was solved: 1.7 trillion unknowns.

With **Monte Carlo** we sample the physics of every single interaction of every single particle until we have enough samples to assert that something is statistically valid. Thie requires lots and lots of samples, but is typically fairly easy to parallelize.

	Monte Carlo	Deterministic
Strengths	* General geometry * Continuous Energy * Continuous in Angle * Inherently 3-D * Easy to parallelize on CPUs	* Fast * Global Solution * Solution is of same quality everywhere
Weaknesses	* Slow * Might be memory intensive * Solutions have statistical error * Local solutions only * Must adequately sample phase space * Need efficient VR	* Variable discretization governs solution quality * Might be memory intensive * Solution contains truncation error * Constrained by what you can mesh * Ray Effects * Can be complicated to parallelize on CPUs