Computational methods for nuclear engineering

Workshop on Computational Nuclear Science and Engineering

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IAEA

2021-07-12

About me

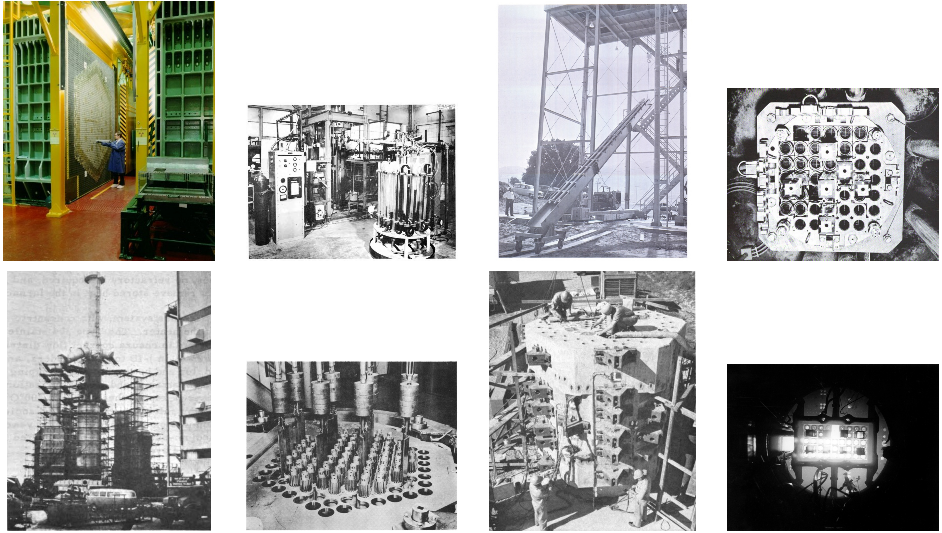
- Started programming on an Osborne 1 in childhood
- Nuclear engineering Ph.D. from University of Michigan
- Been working at TerraPower, LLC since 2009
- Core design, fast reactor physics, software, business
- P.E. in State of WA in 2019
- Current role: Manager of Digital Engineering
- On the side: I run whatisnuclear.com

Me and Waffles, several months ago

Technical questions needing answers in nuclear engineering

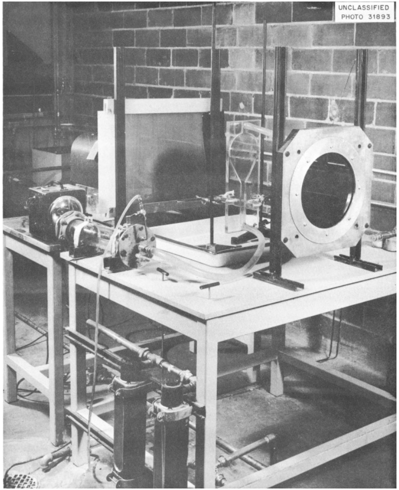
- **Radiation transport** Where are the neutrons and photons? Where are they headed? How fast are nuclei splitting? What power are they generating, and where?
- **Thermal/hydraulics** How fast must we flow coolant to carry away the heat? What are the resulting pressures and vibrations?
- **Fuel performance** What are the mechanical and chemical dynamics of fuel system given the nuclear reactions and irradiation?
- **Mechanical** What are the mechanical loads, dynamics, and vibrations amongst the fuel assemblies and/or other structures?
- **Plant systems** How do the pumps, pipes, heat exchangers, instrumentation, etc. perform in expected and postulated on- and off-normal conditions?

Experiments and observations form the initial answers

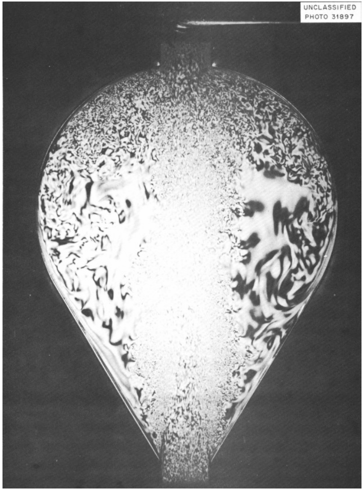


Some historical nuclear experiments

Scale models can be considered analog computers

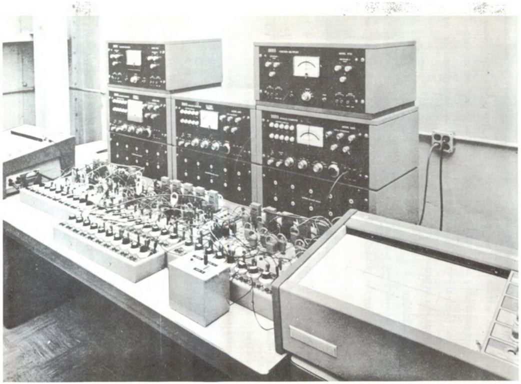


This rig takes pictures through a special plexiglass analog of the HRE vessel

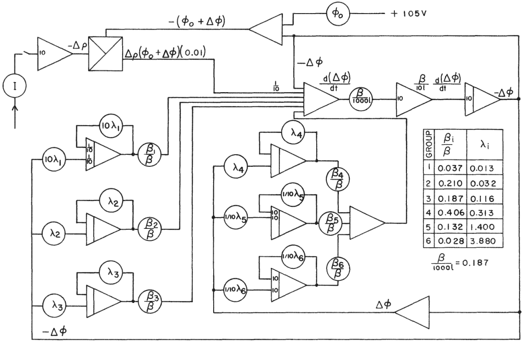


Flow patterns due to flow double refraction appear in a Milling-Yellow solution

Analog computer to measure the power coefficient of reactivity



Analog computer at Hallam



GROUP	$\frac{\beta_i}{\beta}$	λ_i
1	0.037	0.013
2	0.210	0.032
3	0.187	0.116
4	0.406	0.313
5	0.132	1.400
6	0.028	3.880

The schematics

https://babel.hathitrust.org/cgi/pt?id=mdp.39015095040682&view=1up&seq=32

Nuclear engineers were some of the first major users of digital computers

The development program for the experimental breeder reactor No. 2 is now well under way. The complex physics problems that arise in fast reactors are being solved on the UNIVAC electronic computer at New York University. Reactor physics measurements required for the program were made with a subcritical core assembly using the neutron source reactor at the Argonne National Laboratory. These exponential experiments are nearly completed and the data is presently being analyzed by the AVIDAC electronic computer at Argonne.

Digital computers were used in 1955 for reactor design
(https://babel.hathitrust.org/cgi/pt?id=mdp.39015003993188&view=1up&seq=1)

There were dozens upon dozens of nuclear codes in 1964!

TABLE II

THREE-DIMENSIONAL GROUP DIFFUSION THEORY CODES

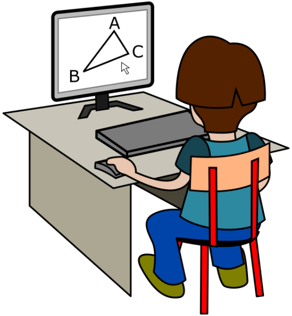
Name	Maximum number: Groups	Maximum number: Points[b]	Materials	Group coupling	References	Computer	Time estimate
FLAME	4	$\frac{230{,}000}{G}$	500	Few	[*4, 97, 125*]	LARC	0.2 msec/point/inner iteration; 3 to 4 hr for 3-group, 50,000-point problem.
TKO-1	4	4750	511	Few	[*95, 126–128*]	704	2.5 msec/point/inner iteration; 2.7 hr for a 2-group, 10,000-point problem.
TNT	4	100,000	150	Few	[*99, 122*]	S-2000	0.8 msec/point/inner iteration 6 to 10 hr for 3-group, 6200-point problem.
TRIXY	—	$\frac{150{,}000}{G}$	100	Few	[*129*]	704	
UFO	5	30,000-7Q	512	Few	[*130, 131*]	704	12 to 15 min/source iteration for 12,000-point, 3-group problem.
WHIRLAWAY[a]	2	12,750	100	Few	[*132–135*]	7090 FORTRAN	6 msec/point/iteration; $1\frac{1}{2}$ to 4 hr for 10,000-point problem.

[a]Available through the Argonne Code Center
[b]G represents the number of groups; Q represents the number of point types.

From Elizabeth Cuthill - Digital Computers in Nuclear Reactor Design, 1964
(`https://doi.org/10.1016/S0065-2458(08)60356-3`)

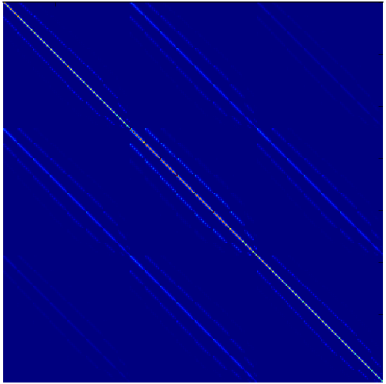
Today, computation is used for a variety of aims

- General engineering/design without the challenges of classical analysis
- Run many perturbed cases to seek a multi-objective optimum
  - in trade studies backing design decisions
  - in preparation for targeted experiments
  - to estimate complex system-level sensitivities
- Explore a new space in reactor design
- Seek insight into some complexity with ultra-high fidelity



Basic approach to deterministic computational nuclear engineering

- Write a balance statement
- Specify boundary conditions
- Make assumptions to simplify as necessary
- Discretize the solution space considering geometry and material properties
- Cast balance statement into matrix form
- Solve matrix equation numerically
- Provide results in intuitive and useful way



Neutronics

The Neutron Transport Equation is a balance statement

$$\left(\frac{1}{v(E)}\frac{\partial}{\partial t} + \hat{\mathbf{\Omega}}\cdot\nabla + \Sigma_t(\mathbf{r},E,t)\right)\psi(\mathbf{r},E,\hat{\mathbf{\Omega}},t) =$$

$$\frac{\chi_p(E)}{4\pi}\int_0^\infty dE'\,\nu_p(E')\,\Sigma_f(\mathbf{r},E',t)\,\phi(\mathbf{r},E',t) + \sum_{i=1}^{N}\frac{\chi_{di}(E)}{4\pi}\lambda_i C_i(\mathbf{r},t) +$$

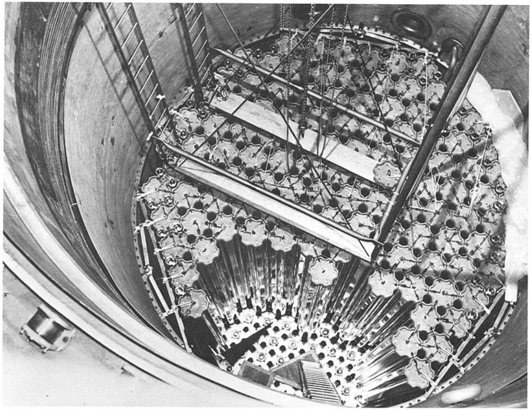
$$\int_{4\pi} d\Omega' \int_0^\infty dE'\,\Sigma_s(\mathbf{r},E' \to E,\hat{\mathbf{\Omega}}' \to \hat{\mathbf{\Omega}},t)\psi(\mathbf{r},E',\hat{\mathbf{\Omega}}',t) + s(\mathbf{r},E,\hat{\mathbf{\Omega}},t)$$

The neutron transport equation

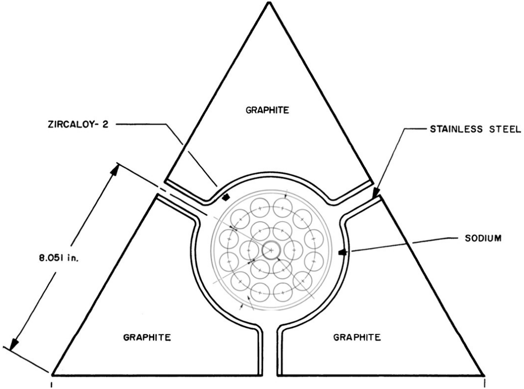
Given a solution to this, you get nuclear reaction rates, which give:

- Gamma source distribution (leads to another transport solve)
- Power distribution (cooling, distortions)
- Dose rate distribution (material damage, detector signal)
- Dynamics (operations, safety)

The domain: a nuclear core

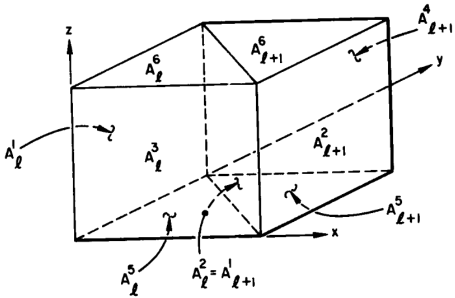


The Hallam core

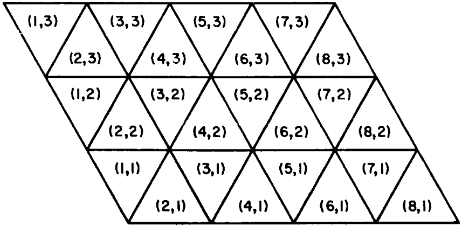


A large 'unit cell'

Spatial discretization



A Triangular-Z volume element



A 120° domain

From DIF3D: A Code to Solve One-, Two-, and Three-Dimensional Finite-Difference Diffusion Theory Problems

Some approximations to the transport equation

Steady state, multi-group diffusion:

$$(D_g + \Sigma_g)\,\phi_g - \sum_{g' \neq g} T_{gg'}\phi_g = \frac{1}{\lambda}\chi_g \sum_{g'=1}^{G} F_{g'}\phi_{g'}, \tag{1}$$

$$M = \begin{bmatrix} [A_1] & & & [0] \\ & [A_2] & & \\ & & \ddots & \\ [0] & & & [A_G] \end{bmatrix} - \begin{bmatrix} [0] & [T_{12}] & \cdots & \cdots & [T_{1G}] \\ [T_{21}] & [0] & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \left[T_{G-1,G}\right] \\ [T_{G1}] & [T_{G2}] & \cdots & \left[T_{G,G-1}\right] & [0] \end{bmatrix}, \tag{2}$$

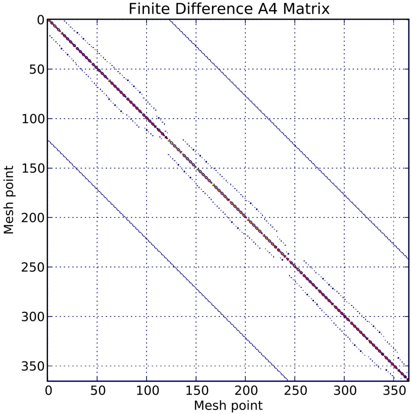
Eigenvalue equation:

$$M\phi = \frac{1}{\lambda}B\phi, \tag{3}$$

Building the matrices

$$A_g = \begin{bmatrix} \ddots & \ddots & & \ddots & & & \\ & \left[A_{gx}^{J-1,k}\right] & \left[A_{gy}^{J,k}\right] & & \left[A_{gz}^{J-1,k+1}\right] & & \\ & & \left[A_{gx}^{J,k}\right] & [0] & & \left[A_{gz}^{J,k+1}\right] & \\ & & & \left[A_{gx}^{1,k+1}\right] & \left[A_{gy}^{2,k+1}\right] & & \ddots \\ & & & & \ddots & \ddots & \end{bmatrix}, \tag{4}$$

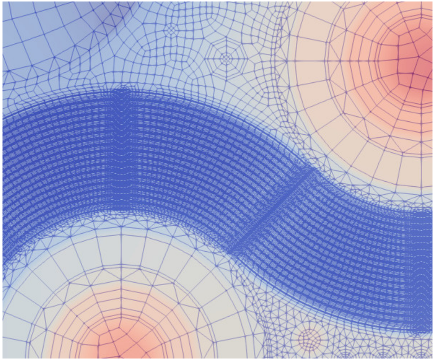
$$\left[A_{gx}^{j,k}\right] = \begin{bmatrix} b_1 & -a_2^x & & & & & \\ -a_2^x & b_2 & -a_3^x & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & -a_{I-1}^x & b_{I-1} & -a_I^x \\ & & & & & -a_I^x & b_I \end{bmatrix}_{ikg}, \tag{5}$$



A 7-banded diffusion matrix for one group in 1/3-core 3D triangular geometry

We have high fidelity deterministic codes these days

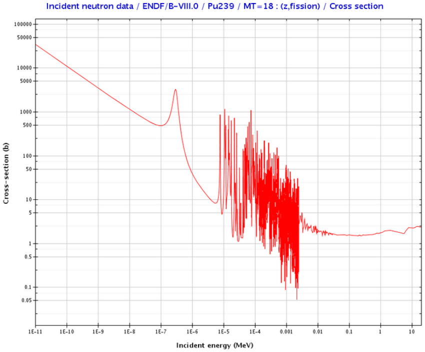
- Unstructured mesh
- Detailed treatment of scattering
- Requires cross section averaging lattice calculations
- Powerful, iterative matrix solvers (e.g. LAPACK, PETSc, Trilinos)



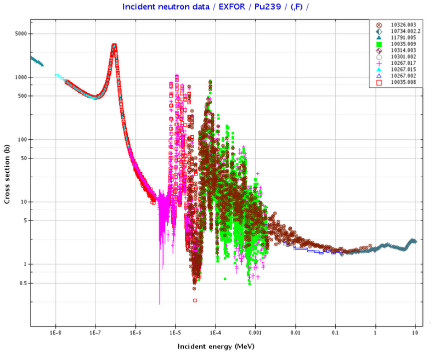
A fine mesh of the ATR from
`https://rattlesnake.inl.gov/SitePages/Home.aspx`

Nuclear data evaluations underly transport models

- Many measurements are made
- Nuclear models run to interpolate between data
- Complex statistics and Bayesian inference to get 'best' fit



The evaluated data

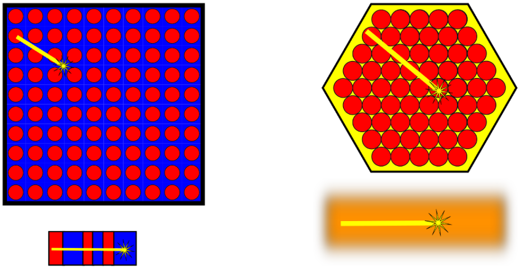


A small selection of experimental data

https://www.oecd-nea.org/janisweb

Averaging cross sections across regions and energies is a complex art

- Strong resonances from one nuclear depress flux, impact averaging of others
- Spatial details vs. spectral details matter differently depending on composition
- Nearby assemblies can impact the averaging as well
- Many lattice codes are specialized for a subset of reactor designs



A LWR Assembly

A SFR Assembly

What slow neutrons see vs. fast neutrons

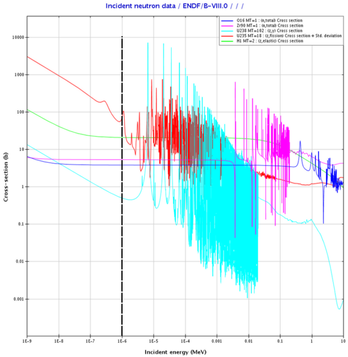
Monte Carlo: explicitly track particle histories

- No geometry approximations
- No angular approximations
- No multi-group approximations
- No cross section averaging
- **But...** lots and lots of histories needed
- Big computers
- Lots of time

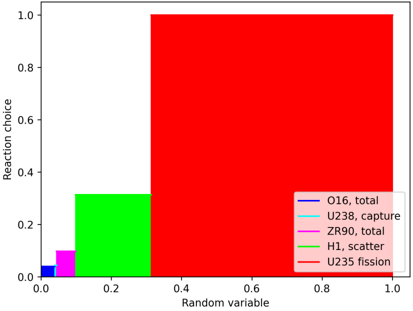
The Monte Carlo Casino (CC-BY-2.0 Lolipouette)

Monte Carlo: basics

- Roll dice: sample distance to next interaction
- Sample from cross section data to choose reaction
- Sample from cross section data to choose outgoing energy and direction
- Repeat billions of times, tallying up track length & reaction rates



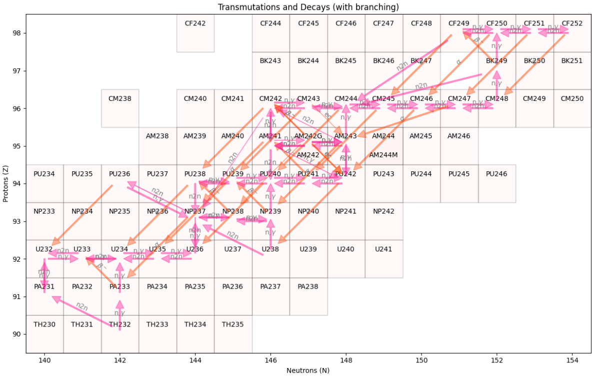
Look at the macroscopic cross sections at the particle's current energy



A discrete CDF for material choice

Transmutation and decay

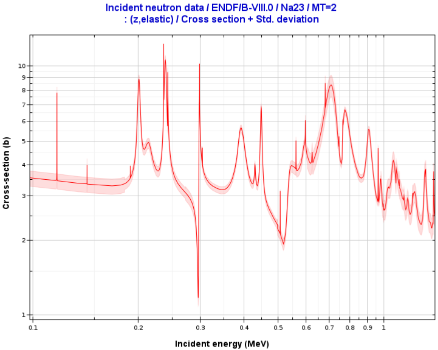
$$\frac{\partial N_i}{\partial t} = -N_i\left(\sum_{g=1}^{G}\sigma^i_{a,g}\phi_g + \lambda_i\right) + \sum_{j=1}^{I} N_j\left(\sum_{g=1}^{G}\left(\gamma_g^{j\to i}\phi_g\right) + \lambda_{j\to i}\right), \qquad (6)$$

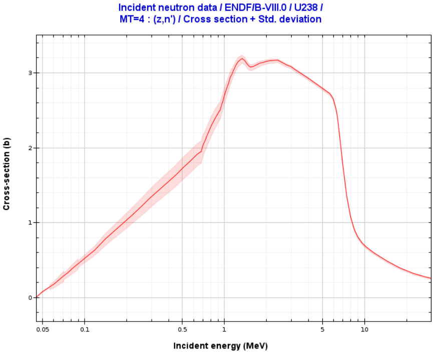


Solution: $N(t) = e^{At}N(0)$

A warning about limitations

- Underlying data have uncertainties! Keep track of them.
- The value of drilling down to 0.5 pcm without a specialized application in mind is dubious when there's 200-500 pcm data uncertainty



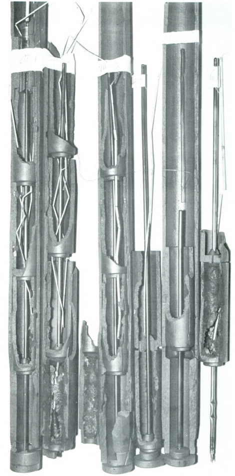


`https://www.oecd-nea.org/janisweb`

Fluid flow and heat transfer

Fluid flow and heat transfer

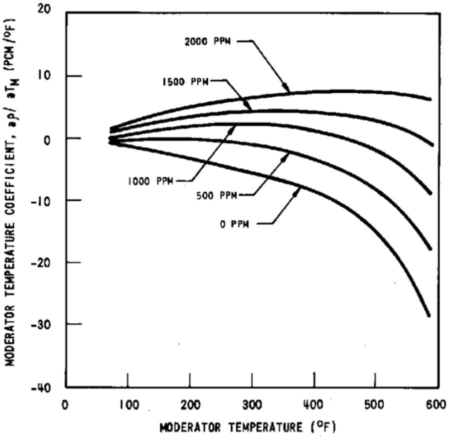
- Fundamental to safety performance: need to keep components at safe temperatures and pressures
- Important to economics: attempt to safely get more power out of same equipment
- Often strongly coupled to neutronics



Some (intentionally) overheated fuel pins `https://babel.hathitrust.org/cgi/pt?id=mdp.39015078511006&view=1up&seq=45`

Important couplings between thermal/hydraulics and neutronics

- Macroscopic nuclear cross sections are temperature dependent (thermal expansion, soluble boron)
- Microscopic nuclear cross sections are temperature dependent (Doppler effect)
- Flow-induced pressure can distort the core, causing changes in macroscopic cross section
- In fluid fuel reactor or severe accidents, flow moves the fuel and delayed neutron precursors



The Moderator Temperature Coeff in a PWR (Joseph M. Farley FSAR Fig. 4.3-30) `https://www.nrc.gov/docs/ML0818/ML081820242.pdf`

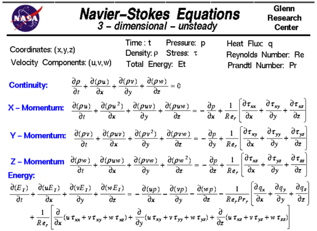
Thermal/Hydraulics Fundamentals

Approach is familiar: discretize spatially, make assumptions and simplifications, cast to matrix looking up material properties, and solve

Governing equations: Navier-Stokes

- Conservation of mass
- Conservation of energy
- Conservation of momentum

These, plus complex fluid property lookup tables (e.g. steam tables) make T/H calculations particularly conducive to computerization



Navier–Stokes Equations
3 – dimensional – unsteady

Glenn Research Center

Coordinates: (x,y,z)
Velocity Components: (u,v,w)
Time : t
Density: ρ
Total Energy: Et
Pressure: p
Stress: τ
Heat Flux: q
Reynolds Number: Re
Prandtl Number: Pr

Continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$

X – Momentum:

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{1}{Re_r}\left[\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z}\right]$$

Y – Momentum:

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} = -\frac{\partial p}{\partial y} + \frac{1}{Re_r}\left[\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z}\right]$$

Z – Momentum

$$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho uw)}{\partial x} + \frac{\partial(\rho vw)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{Re_r}\left[\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}\right]$$

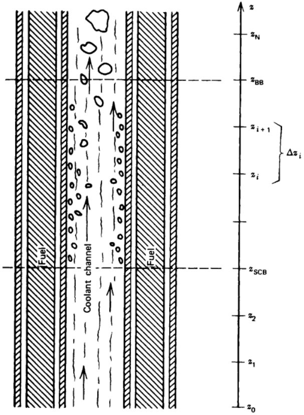
Energy:

$$\frac{\partial(E_T)}{\partial t} + \frac{\partial(uE_T)}{\partial x} + \frac{\partial(vE_T)}{\partial y} + \frac{\partial(wE_T)}{\partial z} = -\frac{\partial(up)}{\partial x} - \frac{\partial(vp)}{\partial y} - \frac{\partial(wp)}{\partial z} - \frac{1}{Re_r Pr_r}\left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right]$$
$$+ \frac{1}{Re_r}\left[\frac{\partial}{\partial x}(u\tau_{xx} + v\tau_{xy} + w\tau_{xz}) + \frac{\partial}{\partial y}(u\tau_{xy} + v\tau_{yy} + w\tau_{yz}) + \frac{\partial}{\partial z}(u\tau_{xz} + v\tau_{yz} + w\tau_{zz})\right]$$

The conservation equations

Hot channel T/H codes

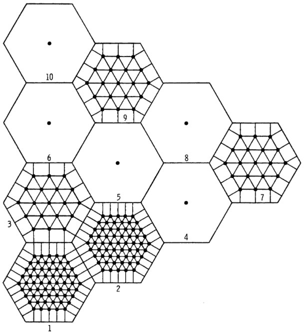
- 1-D fluid flow
- Hot channel factors and correlations for peaking, turbulent mixing, heat transfer, friction factor, and phase slip
- Single phase (liquid metal, molten salt, or gas) or two phase (water)
- 1- or 2-D conduction models into fuel and structures
- Full-core transient calculations trivial



1-D discretization of a single channel https://deepblue.lib.umich.edu/handle/2027.42/89079

Subchannel T/H codes

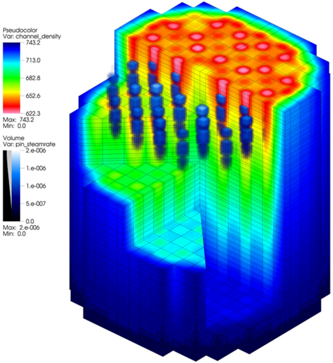
- Typically still 1-D fluid flow
- Communicating subchannels (mixing, conduction)
- Intra-assembly heat transfer, often 3-D conduction to fuel
- Less reliant on hot channel factors, but still need correlations
- Single phase or two phase
- Full-core static calculations routine, transients doable
- Requires pin-level power distributions



Subchannels from CORTRAN `https://www.osti.gov/servlets/purl/6881496`

Typical subchannel code physics

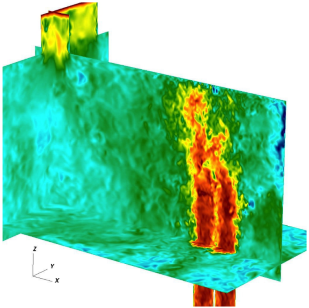
- Steady state and transient solvers
- Single and two-phase flow models with non-uniform channel friction, subcooled voids, etc.
- Turbulent mixing
- Crossflow
- Equation of state for various coolants
- Grid spacer, wire wrap, blocked crossflow
- Axial and radial heat conduction into fuel
- Axial and radial heat conduction in fluid



Subchannel results in Watts Bar 1 from CTF at ORNL
`https://www.ornl.gov/division/rnsd/projects/ctf`

Computational Fluid Dynamics

- High-resolution mesh
- Several methods with different turbulence models
- Multi-phase flow still under development
- Used to verify use of correlations in faster subchannel codes
- Used for thermal striping, stratification, etc.
- Used during trade studies
- Useful in exploring and understanding new design space lacking in experiments
- Helps design the most impactful experiments



Obabko, 2015 https://www.mcs.anl.gov/papers/P5386-0715.pdf

Trivial T/H solution for 1-D single-phase flow

```
def computeIdealizedFlow(a):

    coolants = a.getComponents(Flags.COOLANT)

    tempAvg = (outletInC + inletInC) / 2.0
    coolantProps = coolants[0].getProperties()
    heatCapacity = coolantProps.heatCapacity(Tc=tempAvg)

    deltaT = outletInC - inletInC
    massFlowRate = a.calcTotalParam("power") / (deltaT * heatCapacity)
    return massFlowRate
```

Compute the required mass flow rate given the assembly power

```
def computeAxialCoolantTemperature(a, massFlow):
    """Compute block-level coolant inlet/outlet/avg temp and velocity."""
    # solve q''' = mdot * Cp * dT for dT this time
    inlet = inletInC
    for b in a:
        b.p.THcoolantInletT = inlet
        coolant = b.getComponent(Flags.COOLANT)
        coolantProps = coolant.getProperties()
        heatCapacity = coolantProps.heatCapacity(Tc=inlet)
        deltaT = b.p.power / (massFlow * heatCapacity)
        outlet = inlet + deltaT
        b.p.THcoolantOutletT = outlet
        b.p.THcoolantAverageT = (outlet + inlet) / 2.0
        # V [m/s] = mdot [kg/s] / density [kg/m^3] / area [m^2]
        b.p.THaveCoolantVel = (
            massFlow
            / coolantProps.density(Tc=b.p.THcoolantAverageT)
            / coolant.getArea()
            * 100 ** 2
        )
        inlet = outlet
```

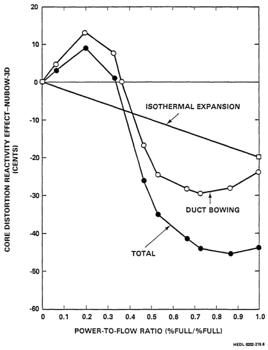
Given mass flow rate, compute the axial coolant temperature distribution

Core Mechanical

Core Mechanical Analysis

Understanding how the fuel assemblies interact with the support structures

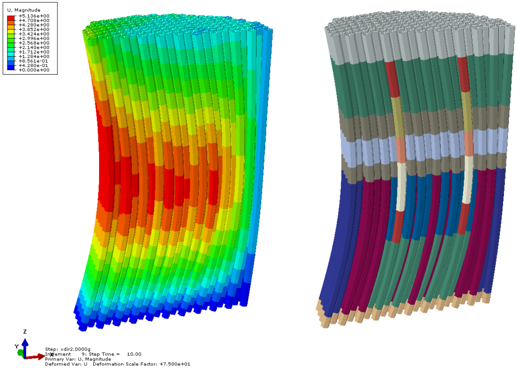
- Seismic analysis important for safety
- Vibrations can cause premature fuel failure
- Fuel management loads needed for reload operations
- Core distortions can have large impacts on the safety case in some reactors



Core radial expansion's impact on FFTF reactivity
https://www.osti.gov/servlets/purl/5236450

The Finite Element Method

- Works well with highly complex shapes
- Governing equations: $F = ma$ and $\sum F = 0$
- Matrix size is proportional to the mesh resolution



A model of a core subjected to an acceleration (from TerraPower LLC)

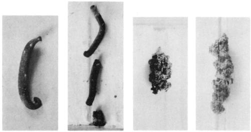
Fuel Performance

Fuel Performance

Reliable prediction of fuel behavior in normal and off-normal conditions.

- Important for safety and operations-related issues like fission product retention
- Tied to fuel thermal and burnup limits and therefore economics and sustainability
- Typically computes temperature, stress, strain, fission gas pressure, fission gas release, cladding corrosion, and cladding erosion within a fuel pin/clad system
- Arguably should include fuel salt chemistry models for fluid fuel

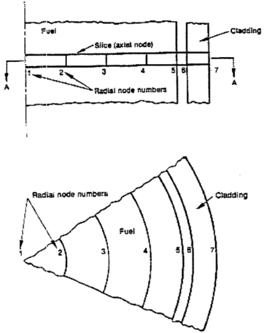
Fresh fuel pellets



Irradiated fuel slugs (from the olden days)
https://www.osti.gov/servlets/purl/4300801

Fuel Performance computational approach

- Inherently dependent on difficult-to-measure correlations e.g. for burnup-dependent properties
- Beware overfitting the experimental data
- Historical codes use several hundred mesh points and run in seconds on a modern PC
- Solves solid mechanics statics/dynamics equations including irradiation strain models using finite difference or finite element methods
- Several modern codes make fine-mesh problems and can leverage supercomputers

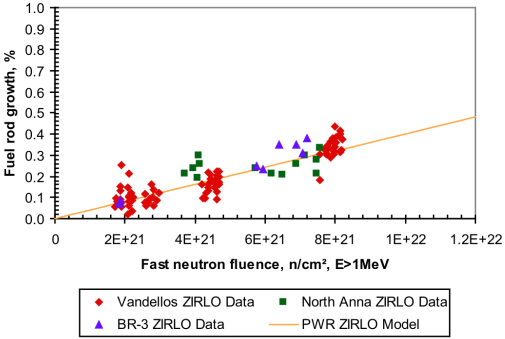


A typical FRAPTRAN computational mesh
https://www.nrc.gov/docs/ML0125/ML012530260.pdf

Fuel Performance computational approach

Couplings

- Fission gas release and axial/radial strain can seriously impact neutronics in many cases
- Coupling with thermal/hydraulics provides fuel temperature limits
- Clad strain can impact coolant flow
- For fluid fuel, coupling with neutronics is fundamental

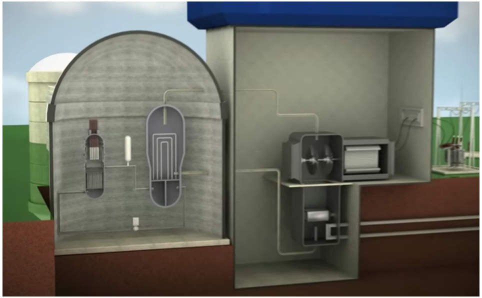


Fuel performance correlations from FRAPTRAN
https://fast.labworks.org/file-download/download/public/108

Systems codes

Systems codes

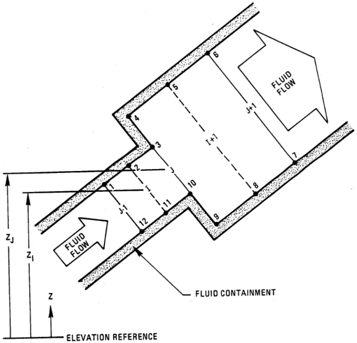
- Simulate the entire plant in various operational and off-normal conditions
- Front and center in licensing
- Includes representations of major equipment in balance of plant (sometimes in lower fidelity than the core)



Plant systems in a PWR

Simple discretization lumped-parameter models

- Coolant property lookup tables
- Includes or is heavily informed by subchannel code and fuel performance code
- Includes point or spatial kinetics nuclear models
- Simple models are conducive to running many hundreds of cases to support the licening basis
- Experimental validation sometimes easier when simple and conservative
- Handle varying degrees of severe accident

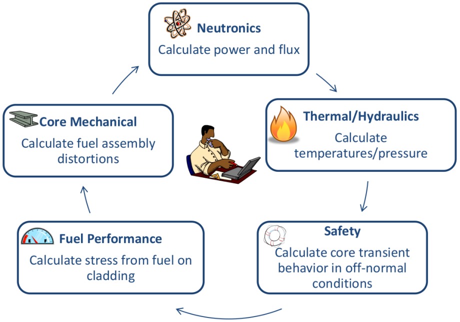


Discretization in TOPAZ
https://www.osti.gov/servlets/purl/5437631

Information Management

Multiphysics analysis suites

- Automate time-consuming analysis workflows
- Capture important coupled physics effects for complex analyses
- Write full analysis methodologies as code (with rigorous QA)
- Leverage multiobjective optimization systems
- Machine learning, AI, digital twin, etc.



A person (or supercomputer) running full-scope calculations rapidly

Project and Asset Information Management

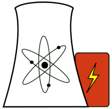
- Indirect costs are now 50% of new nuclear costs!
- Inefficiencies in high-level work process are ripe for disruption
- Computers as information management and process facilitators
- See: IAEA-TECDOC-1651, EPRI 3002003126, and cmbg.org.

A data hub for nuclear enterprise
https://www-pub.iaea.org/MTCD/Publications/PDF/te_1651_web.pdf

Conclusions

- Computers have been and will remain incredible tools for nuclear engineers
- Each area has still-relevant methods (and in some cases codes!) from the 1980s and extraordinary high-fidelity modern codes for specialized applications
- This only barely scratches the surface; dozens of publications per month
- The magnitude of mechanical, civil/structural, electrical, and operations engineering at nuclear plants hasn't even been mentioned
- There are parts of the nuclear enterprise that have not yet fully leveraged computers

Discussion!



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