The concept of space is not quite so overwhelming if you consider that: **No matter where you go, there you are!**

CHAPTER 6
TWACKING THROUGH A PLETHORA OF CORNUCOPIA

OR

Browsing through the field with the intention of locating the meadow muffins so that, when you have to make tracks later, they are not dark brown.

OR

How to drain swamps and avoid alligators.

At this point, we will try to put the popular space time computational methods on a family tree. This will help to keep things straight when we are whipping around for a method to solve our problem. Equally important, it will help us avoid misusing the methods that we do finally choose. For further reference in the field, we should know, by the end of this chapter, all the basic things we need to understand the [illegible] about any space or space-time [illegible], 1) how it [illegible], 2) how to place it on the family tree and 3) assess the good and bad points, assumptions, etc.

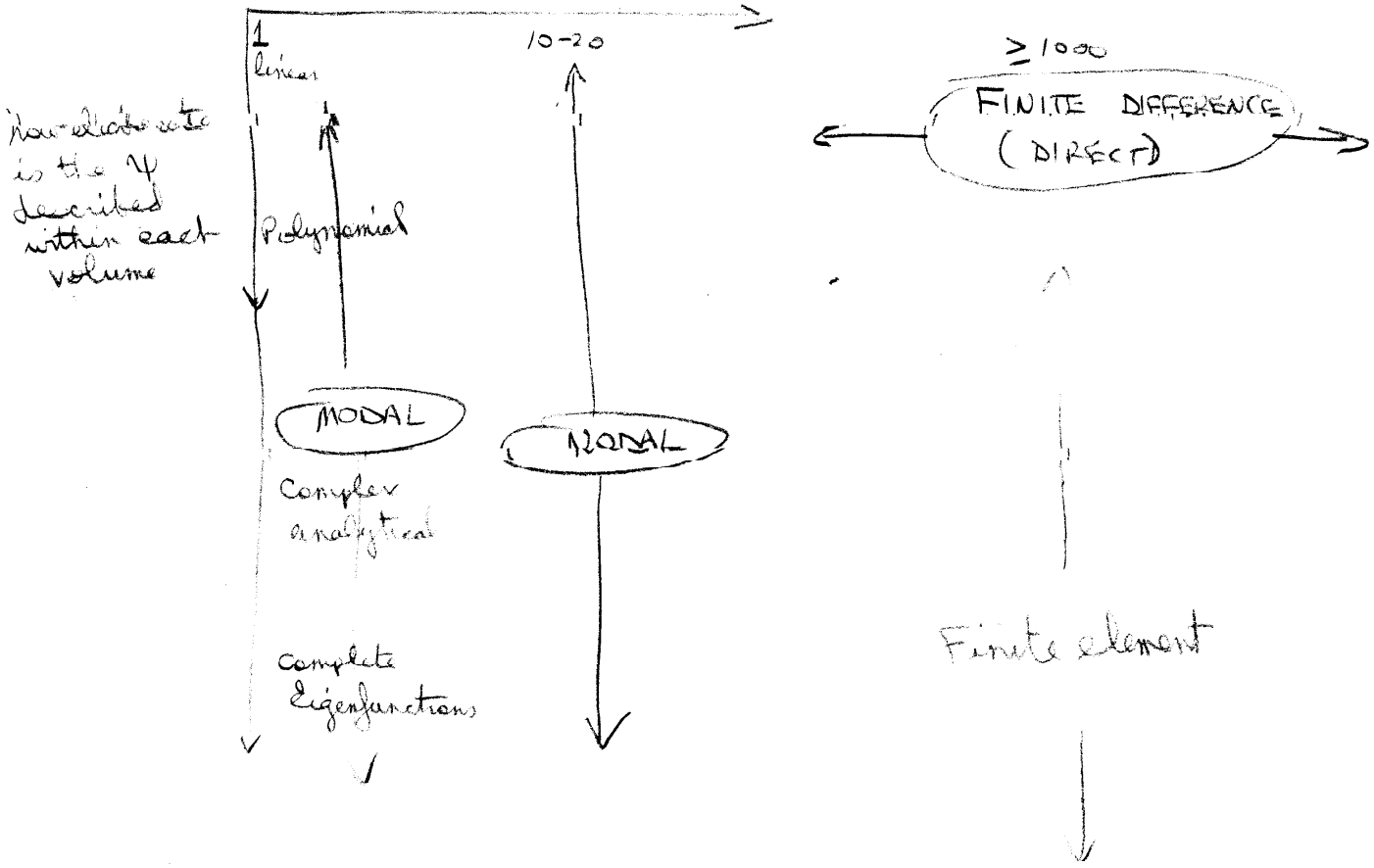
In Hetrick's book (reference 1), Henry gives an overview of the field. I've condensed his overview on figure 6-1. His whole paper, pp 9-21 is well worth reading.

I guess people like to put things in specific categories; it is convenient. But, at the same time, it can be stifling because it tends to obscure the links and similarities between all these methods.

In my opinion, the categories arise basically because of the way the space component is handled. There are really only two aspects, or two space issues which describe all the categories:

how many volumes is the core divided up into?

how elaborate is the ψ described within each volume



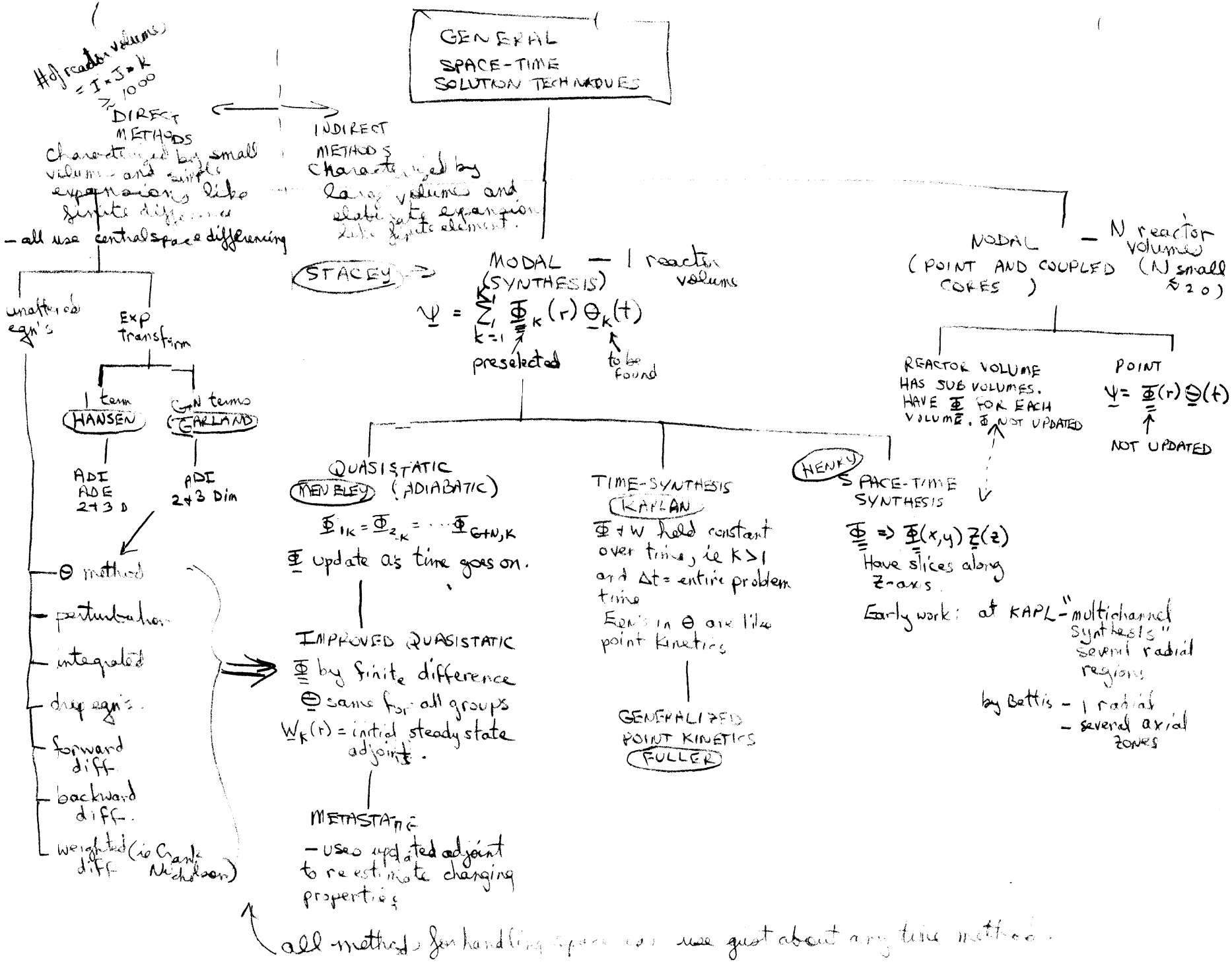

GENERAL SPACE-TIME SOLUTION TECHNIQUES
# of reactor volumes = I*J*K ≥ 1000
DIRECT METHODS
Characterized by small volumes and simple expansions like finite differences
- all use central space differencing
INDIRECT METHODS
Characterized by large volumes and elaborate expansions like finite elements
STACEY
MODAL (SYNTHESIS) — I reactor volumes
$\Psi = \sum_{k=1}^{K} \underline{\underline{\Phi}}_k(r)\,\Theta_k(t)$
preselected
to be found
NODAL (POINT AND COUPLED CORES) — N reactor volumes (N small ≲ 20)
REACTOR VOLUME HAS SUB VOLUMES. HAVE $\underline{\underline{\Phi}}$ FOR EACH VOLUME. $\underline{\underline{\Phi}}$ NOT UPDATED
POINT
$\Psi = \underline{\underline{\Phi}}(r)\,\Theta(t)$
NOT UPDATED
unaffected eqn's
Exp transform
1 term
HANSEN
ADI ADE 2+3 D
G+N terms
CARLAND
ADI 2+3 Dim
Θ method
perturbation
integrated
drop eqn's
forward diff.
backward diff.
weighted (ie Crank Nicholson)
QUASISTATIC
MENELEY (ADIABATIC)
$\underline{\underline{\Phi}}_{1K} = \underline{\underline{\Phi}}_{2K} = \cdots \underline{\underline{\Phi}}_{G+N,K}$
$\underline{\underline{\Phi}}$ update as time goes on.
IMPROVED QUASISTATIC
$\underline{\underline{\Phi}}$ by finite difference
Θ same for all groups
$W_K(r)$ = initial steady state adjoint.
METASTATIC
- uses updated adjoint to re-estimate changing properties
TIME-SYNTHESIS
KAPLAN
$\underline{\underline{\Phi}}$ & W held constant over time, ie K>1 and Δt = entire problem time
Eqn's in Θ are like point kinetics
GENERALIZED POINT KINETICS
FULLER
HENNY
SPACE-TIME SYNTHESIS
$\underline{\underline{\Phi}} \Rightarrow \underline{\underline{\Phi}}(x,y)\,\underline{Z}(z)$
Have slices along z-axis
Early work: at KAPL - "multichannel synthesis" several radial regions
by Bettis - 1 radial
- several axial zones
all methods for handling space can use most about any time method.

FIGURE 6-1

see, for instance, in Hetrick's book (ref 1), Henry p 14 + Hansen p 165-166

There seems to be an ongoing battle as to the best approach. Stacey and Hendry are the upholders of the synthesis (modal) and nodal schools while Hansen believes the best approach is the finite difference approach. Let's summarize the relative merit:

Finite Difference
- slow + expensive
- can estimate error by truncation analysis
- used for kernel marking
- flexible
- can easily change Ψ eqn's without changing technique much.
- don't need much intuition.

Modal and nodal
- fast + cheap
- need lots of intuition to choose Φ
- can be used to generate insight into harmonics of Ψ.
- method of generating flux and volume averaged parameters are in dispute.
- no error estimate available.

In the limit, as more variations on old themes hit the marketplace, a continuum of techniques forms. For instance, as higher order approximations are used in finite difference techniques, we approach finite elements. If the finite element volumes were made larger, we move towards nodal techniques. Likewise if you have a modal technique and simplify the elaborate

- scheme to find $\vec{F}$, Θ, etc, and apply it over smaller volumes, you move into nodal and eventually into finite difference techniques.

Now, if you throw in all the possible time solution schemes, you end up with countless variations on a theme. Of course, each investigator of scheme X, or should I say XYZET, claims superior results with his or her method.

at this point in time I would recommend the consumer to buy (was a first purchase) a good used clunker which will always crank ever even on the coldest morning. Pick a nice stable, central differenced in space, weighted differenced in time (or some variant thereof) general G+N, 1, 2+, D package that has good I/O including graphics. As an essential extra you'd need a good property library which will do group integration or collapsing of general energy dependent cross sections. You should look for one that will allow interfacing with a thermal hydraulics package. Nothing fancy, but it will probably beat the pants off the competition when evaluated on the basis of overall ability to get the total job done from start to finish within a tight, preset job time (including, problem definition, equation setup, programming debugging, report writing, error analysis, etc.). If you pick one that has an exponential transformation in time using the dominant eigenvalue and one that satisfies the "strongly A-stable" criteria,

- tion you may get quite acceptable performance in terms of Δt's.

Do time goes on, you may miss the need to pick up one of the modal or nodal methods. They are faster, running but tend to be trickier and are more fickle. But by this time you've gained some experience in the field so that you'll know pick the Φ, etc. appropriate for your problem and you always have your clunker to benchmark against.

Let's take a closer look at some of the more favored methods.

DIRECT (finite difference) as per Hansen section p165 of Ref 1.

- → WIGLE, a 1-D code and TWIGLE, its 2-D cousin to space, are implicit based codes which use the following algorithm:

$$\underline{\underline{A}} = \underline{\underline{A}}_1 + \underline{\underline{A}}_2$$

$$\frac{\underline{\Psi}^{j+1} - \underline{\Psi}^{j}}{\Delta t} = \underline{\underline{A}}_1 \underline{\Psi}^{j+1} + \underline{\underline{A}}_2 \underline{\Psi}^{j} \quad , \; j \Leftrightarrow \text{time slice}$$

$$\text{or} \quad \underline{\Psi}^{j+1} = \left[\underline{\underline{I}} - \Delta t \, \underline{\underline{A}}_1\right]^{-1} \left[\underline{\underline{I}} + \Delta t \, \underline{\underline{A}}_2\right] \underline{\Psi}^{j} \qquad 6\text{-}1$$

the truncation error is given as:

$$(T.E.) = \frac{\Delta t^2}{2}\left[\underline{\underline{A}}^2 - 2\underline{\underline{A}}_1\underline{\underline{A}}\right] + \frac{\Delta t^3}{6}\left[\underline{\underline{A}}^3 - 6\underline{\underline{A}}_1^2\underline{\underline{A}}\right] + O(\Delta t^4)$$

- If $A_1 = A_2 = A/2$ we get Crank-Nicholson.

For 1-D problems this method is attractive since the matrices are easy to invert. For 2 and 3D, it is better to go with iterative methods, (see below).

→ GAKIN — a 1-D code using an exponential transformation:

$$\underline{\Psi}(t) = e^{-\underline{\underline{\Omega}}t}\,\underline{\Theta}(t) \Rightarrow \frac{d\underline{\Theta}}{dt} = e^{-\underline{\underline{\Omega}}t}\left(\underline{\underline{A}} - \underline{\underline{\Omega}}\right)e^{-\underline{\underline{\Omega}}t}\,\underline{\Theta} \qquad \text{6-2}$$

But what is $\underline{\underline{\Omega}}$? How do you choose it?
One popular method is to make it a scalar and select its value based on past history. This has good stability characteristics.
Equation 6-2 is rewritten:

$$\frac{d\underline{\Theta}}{dt} + \left(\underline{\underline{\Gamma}} - \underline{\underline{\Gamma}}\right)\underline{\Theta} = e^{-\underline{\underline{\Omega}}t}\left(\underline{\underline{P}}+\underline{\underline{L}}+\underline{\underline{U}}\right)e^{-\underline{\underline{\Omega}}t}\,\underline{\Theta} \qquad \text{6-3}$$

$\underline{\underline{\Gamma}}$: non-diffusion diagonal; $\underline{\underline{P}}$: diffusion; $\underline{\underline{L}}$, $\underline{\underline{U}}$: upper + lower triangular

Equation 6-3 is then integrated analytically over the time step.

$$\text{Ch. (T.E.)} = -\frac{\Delta t^2}{2}\left[\delta\left(W_0\,\underline{\underline{I}} - \underline{\underline{\Gamma}} - 2\underline{\underline{P}}\right)\right]\underline{U}_0 \qquad \text{6-4}$$

where $\delta = W_0\,\underline{\underline{I}} - \underline{\underline{\Omega}}$ ⇐ nice neat diagonal!

$\underline{U}_0$ = fundamental mode
W_0 = " " eigenvalue.

LUMAC is a 2-D extension of GAKIN. Replace $\underline{\underline{P}}$ by

$$P(x) + P(y) \Rightarrow \underline{\underline{P}}\,\underline{\Psi} = \underline{\underline{P}}(x)\,\underline{\Psi} + B_y^2\,\underline{\Psi} \qquad \text{6-5}$$

(B_y^2: known buckling.)

→ MITKIN - 2-D using alternating-direction explicit (ADE) method:

$$\frac{\underline{\Theta}^{j+1} - \underline{\Theta}^{j}}{\Delta t} = e^{-\underline{\underline{\Omega}}\Delta t}\left[\underline{\underline{A}}_1 + \underline{\underline{Q}}_1 - \underline{\underline{\Omega}}\right]\underline{\underline{R}}^{\underline{\underline{\Omega}}\Delta t}\,\underline{\Theta}^{j+1} + e^{-\underline{\underline{\Omega}}\Delta t}\left[\underline{\underline{A}}_2 + \underline{\underline{Q}}_2\right]\underline{\underline{R}}^{\underline{\underline{\Omega}}\Delta t}\,\underline{\Theta}^{j}$$

and

$$\frac{\underline{\Theta}^{j+2} - \underline{\Theta}^{j+1}}{\Delta t} = e^{-\underline{\underline{\Omega}}\Delta t}\left[\underline{\underline{A}}_1 + \underline{\underline{Q}}_1\right]e^{\underline{\underline{\Omega}}\Delta t}\,\underline{\Theta}^{j+1} + e^{-\underline{\underline{\Omega}}\Delta t}\left[\underline{\underline{A}}_2 + \underline{\underline{Q}}_2 - \underline{\underline{\Omega}}\right]e^{\underline{\underline{\Omega}}\Delta t}\,\underline{\Theta}^{j+1}$$

6-6

where $A_1 + Q_1 + A_2 + Q_2 = A$

$Q_1 + Q_2 = P$.

Choose partitioning to make inversion easy, example:

Q = 5 stripe in 2-D ; set Q_1 - lower + ½ diagonal

Q_2 = upper + ½ diagonal

To next algorithm:

$$\underline{\psi}^{j+2} = e^{\underline{\underline{\Omega}}\Delta t}\left[\underline{\underline{I}} - \Delta t\left(\underline{\underline{A}}_2 - \underline{\underline{Q}}_2 - \underline{\underline{\Omega}}\right)\right]^{-1}\left[\underline{\underline{I}} + \Delta t\left(\underline{\underline{A}}_1 + \underline{\underline{Q}}_1\right)\right] \times$$

$$\left[\underline{\underline{I}} - \Delta t\left(\underline{\underline{A}}_1 + \underline{\underline{Q}}_1 - \underline{\underline{\Omega}}\right)\right]^{-1}\left[\underline{\underline{I}} + \Delta t\left(\underline{\underline{A}}_2 + \underline{\underline{Q}}_2\right)\right]e^{\underline{\underline{\Omega}}h}\,\underline{\psi}^{j} = G_1\,\underline{\psi}^{j}\,.$$

6-7

$$(T.E) = \Delta t^2\left[e^{\underline{\underline{W}}_0\Delta t}\left(\delta\,\underline{\underline{A}} + \underline{\underline{\delta}}^2\right)\right]\underline{U}_0$$

Hansen says this is explicit but it sure looks semi-implicit to me (!?!).

On digging into some papers (ref 2, 3 + 4) I found that indeed, MITKIN is semi-implicit but that this particular formulation is called ADE (it is explicit part of the time). By comparison, the ADI method splits the derivation terms into X + Y parts rather than upper and lower part.

-- STKADI - similar to MITKIN except its implicit (!?!) and has a different split for Q.

Hansen then goes through some handwaving on why the (T.E.) is not the be-all and end-all for choosing a method. He argues that one should stay away from methods which partition off just the P part as some other part of time. He says we should keep the transient since we know that the norm

$$\| \underline{\underline{A}}\, \underline{\Psi}^i \| = \left\| \frac{\partial \underline{\Psi}^i}{\partial t} \right\| = \epsilon \text{ where } \epsilon \text{ is small.}$$

That is, the order of magnitude of $\underline{\underline{A}}\, \underline{\Psi}^i$ is small compared to $\underline{\Psi}^i$ and we can't say the same thing about such combinations as $\underline{\underline{P}}\, \underline{\Psi}^i$ etc.

He says that the exponential transformation operates on the full matrix and makes it smaller since we effectively replace $\underline{\Psi}$ with a more slowly varying function $\underline{\Phi}$. He may be right.

But I'm more inclined to think along the lines of the stability analyses that we've done because I did [illegible] and tried a full exponential transformation and got really bad errors. This turned out to be okay if small time steps were required because of rapidly changing fluxes. But stability problems arose just as Devooght predicted because of carrying all the insignificant (large negative) eigenvalues.

MODAL and NODAL

These methods employ:

$$\underline{\Psi} = \sum_{k=1}^{K} \underline{\underline{\Phi}}_k(\underline{r})\underline{\Theta}_k(t) = \sum_{k=1}^{K} \begin{bmatrix} \Phi_{1k} & 0 \\ 0 & \Phi_{2k} \end{bmatrix} \begin{bmatrix} \Theta_{1k} \\ \Theta_{2k} \end{bmatrix} \quad 6-8$$

Substitution into $\frac{\partial \underline{\Psi}}{\partial t} = \underline{\underline{A}}\,\underline{\Psi}$ gives:

$$\sum_{k=1}^{K} \underline{\underline{\Phi}}_k(\underline{r}) \frac{\partial \underline{\Theta}_k(t)}{\partial t} = \sum_{k=1}^{K} \underline{\underline{A}}\, \underline{\underline{\Phi}}(\underline{r})\underline{\Theta}_k(t) \quad 6-9$$

$$\text{or} \quad \underline{\underline{\Phi}}_k(\underline{r}) \frac{\partial \underline{\Theta}_k(t)}{\partial t} = \underline{\underline{A}}\, \underline{\underline{\Phi}}_k(\underline{r})\, \underline{\Theta}_k(t)$$

$$\text{or} \quad \frac{\partial \underline{\Theta}_k(t)}{\partial t} = \left[\underline{\underline{\Phi}}_k(\underline{r})\right]^{-1} \underline{\underline{A}}\, \underline{\underline{\Phi}}_k(\underline{r})\, \underline{\Theta}_k(t) \quad 6-10$$

For each k, we have a weighting function, $\underline{\underline{W}}_k(\underline{r})$.

Equation 6-10 is premultiplied by $\underline{\underline{W}}_k(r) = \begin{bmatrix} W_{1k}(\underline{r}) & 0 \\ 0 & W_{2k}(r) \end{bmatrix}$

and the equation is integrated over the entire reactor volume, leaving K vector equations (of dimension G+N) in K vector unknowns (of dimension G+N).

The variations on the theme give the family tree as shown in Figure 6-1.

A conclusion is the place where you get tired of thinking.

CONCLUSION

Enough written, I think. You should know a meadow muffin when you step in one by now, which was the overall intent of this segment of the course.

Points to contemplate:

1) In light of this course, finish the statement:

"And it goes without saying that ....."

2) What do you think I should have done for this course? Why?

3) What do you think I should do next? Why?

4) How has your thinking on space-time kinetics changed as a result of this course?

5) Could you apply this knowledge elsewhere?

6) ~~Do~~ you think that your [illegible] is in better shape now? You do?! ... What if I told you that all of the above was crap?

It isn't? ← ? → It is?

How do you know? — Maybe I was wrong? Don't you recall that I said Stacey + Hansen made errors, expressed opinions which didn't stand the test of time?

Well, then, let's hear your version.

References

1) Dynamics of Nuclear Fission, D.L. Hill and [illegible], University of Chicago Press, 1972.

2. Reed & Gunn, Nucl. Sci. Eng. 41, p421, 1970

3) Wright, Harmon, Ferguson, Nucl. Sci. Eng, 44, p239, 1971

4) Ferguson, Harmon, Nucl. Sci. Eng. 51, p183, 1972