FUNDAMENTAL CONCEPTS OF MODELLING: The Science of Simulation[1]

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ABSTRACT

This paper addresses the roles of simulation in science and engineering: the extended calculator, the prototyper and the intuition generation medium. Science and engineering involves thought processes which transcend the rational. We admit to the ART of science; simulation offers a means to enhance the practice of this art.

Simulation has emerged as a third wing of science that is orthogonal to experimentation and theory. It has the pedestrian role of the extended calculator in that simulation provides a numerical bridge between symbolic theory and hard experimental data. In this role, discovery has been assisted. But, simulation has proved to be more than a super calculator. The nuclear industry and computational fluid dynamics are but two examples of areas that use simulation to replace experimentation (prototyping) for cost and danger reasons. Further, there is an emerging role of graphics and artificial intelligence in the discovery process. Simulation is clearly becoming not only a tool that reduces the tedium, but one that enhances the creative process.

The paper looks at the state of the art in thermalhydraulics and considers the emerging trends. A general modelling scheme is proposed and a systems view is used to suggest the criteria for 'optimum' simulation models for the working environment.

The basic theme proposed is to reduce the proportion of rational mental time we spend on perspiration so as to allow more time for inspiration non-rational. Our QUEST then is the Quintessential Eureka Stimulator. The QUEST involves the use of existing tools on the micro-computer to enhance problem setup and post-run analysis. The key to successful questing lies, however, in the development of a simulation environment that is seamless through the whole of the process, from problem definition to presentation of results. The framework for this mythical environment is introduced.

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INTRODUCTION: IS SIMULATION A SCIENCE?

What is science? According to 'A dictionary of Philosophy' [FLE79],

> ".... The philosophy of science seeks to show wherein rationality lies...Its theories can be taken to reveal the truth about a hidden objective reality....".

There are problems with this. Science is the domain of rationality but reason is the tool of science. It is rationality seeking to explain rationality. For the working scientist and engineer, however, science is the exploration of verifiable relationships. But how do we conduct a scientific inquiry? By the scientific method, of course, as illustrated in figure 1.

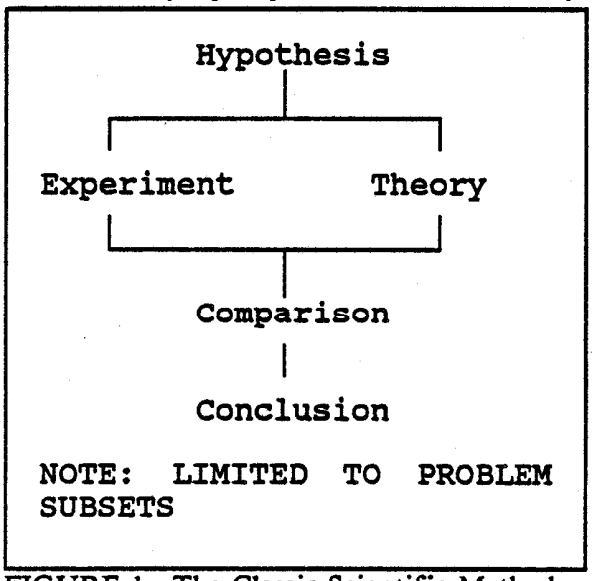

FIGURE 1. The Classic Scientific Method

This is a rational process. But is the actual practical process of carrying out the scientific method totally rational? I say 'No!'. There are simply too many variations on a theme to exhaustively address all possibilities in practical science and engineering problems. To arrive at a tractable (i.e. executable) theory or set of governing equations, MANY assumptions must be made. Experiments entail many approximations. Clearly, decisions have to be made in order to prune the tree of possibilities to a manageable number. And we usually cannot fully justify our decisions other than to say 'the proof of the pudding is in the eating'. Thus the reality of science and engineering involves thought processes which transcend the rational. Our science uses the non-rational (not to be confused with the irrational). This is permissible because, in the end, the results are re-producible and verifiable and, at best, our theories remain simply as working models until something better comes along.

But is it science? Does our work reveal the truth about a hidden objective reality? No, not totally. Our work reveals approximations to the truth about the relationships between objects in our reality, as we conceptualize it. But the scientific method dictates nothing about the way we proceed to hypothesis, theorize and experiment. We can conjure up ideas in any manner. The Scientific Method is simply the process of rational verification. So how do we go about our business? I surveyed my colleagues and found that the creative part, the intuitive, the gut feeling, etc. is usually sudden and unexplainable, and occurs after indepth sustained bull work. One immerses oneself in a problem for an extended period and one day, EUREKA!

Clearly we must now admit to the Art of science, even if it is only 2% of the process, it is essential. It is the guiding light for the train of thought. Carlos Castaneda [CAS77] calls it nagual (the land of the undefined or nonrational) which lies outside the land of the tonal (the land of the defined or rational). The Yin and the Yang. The male and the female. Both exist. One is neither better nor more correct than the other. They simply both are.

This addresses half of the title: Science. Now, where does simulation fit into the picture?

THE NEW ROLE OF SIMULATION: From Science to Simulation

Simulation is neither experimentation in the traditional sense of the word, or theoretical. But clearly, our science and engineering as we now know it would not exist without simulation. Can you conceive of sending a man to the moon without simulation? Or building a nuclear power plant without simulation?

I propose (not originally of course) that there has emerged since the 60's, a new aspect of the scientific method: Simulation, which is orthogonal to experimentation and theory as depicted in figure 2. This new element alters the manner in which we go about our business. Prior to the advent of simulation tools, theories were posed and experiments were performed, often with severe limitations. Theoretical studies are limited by analytical constraints and experiments are limited by the bounds of cost, hazard, and measurement techniques. With simulation, however, analytical work is extended by numerical calculations and experiments are augmented by simulations. Often a simulation is superior to experiments. Some parameters are now more accurately simulated than they can be measured. Full scale simulations are feasible whereas full scale experiments are usually too risky or too costly to do. Not only is the nature of the scientific method changed, but the extent and scope of the method is vastly enhanced.

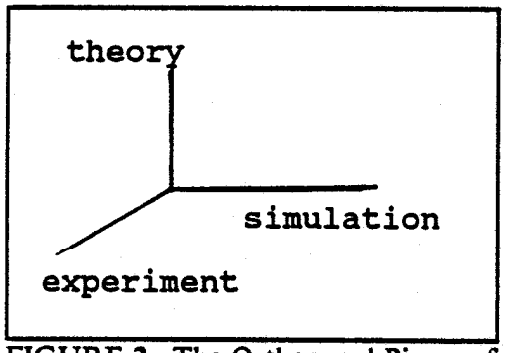

FIGURE 2. The Orthogonal Pieces of the Scientific Method.

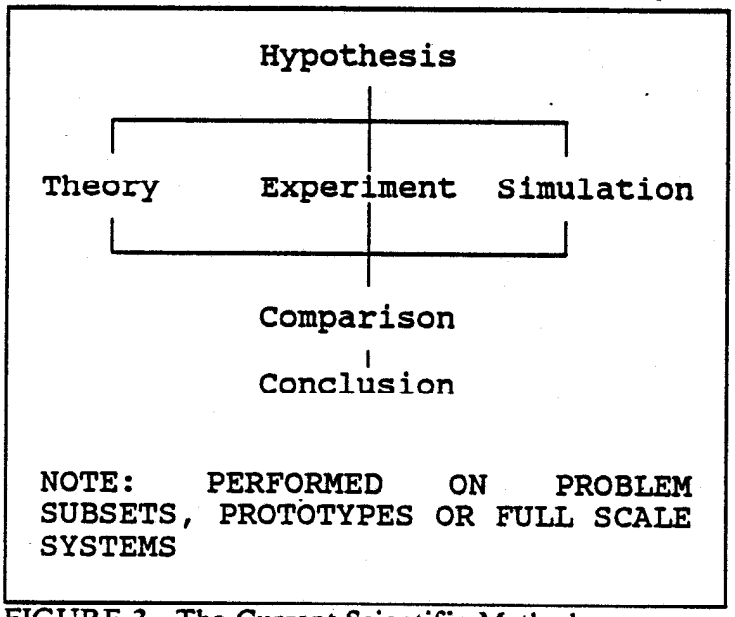

FIGURE 3. The Current Scientific Method.

In general terms, the scientific method as we now perform it is shown in figure 3.This new element warrants a closer look.

The nuclear industry is a typical industry that involves a great deal of fluid processes. It is atypical, however, because one of the processes, the Heat Transport System (HTS), is of critical importance to the safety of the nuclear station. Sustained loss of cooling of the fuel is a catastrophic event. It has to be shown, a priori, that such events are of negligible probability and that the design is adequate to handle all probable events. Adequate design margin must be demonstrated. To compound the difficulty of the task, there is insufficient evidence (thankfully) to base arguments on statistics. Consider also that current designs are pushed to their safe limits in order to extract the maximum power at the minimum cost. A nuclear station can typically cost $\$10^{10}$ (US). A 1% increase in output power can save $\$2 \times 10^{8}$ (US) over the life of the station. The key task of design and analysis of the HTS is, then, is to demonstrate safety, performance, reliability and maintainability prior to the actual construction of the facility. Without

simulation, this clearly would not be possible.

Typically, the simulation support involves the setting up of a large code such as RELAP or RETRAN (or their Canadian equivalents CATHENA and SOPHT). Large data sets are required as input and copious tables of numbers are the result of the many runs that are required. It can take months to acquire the primary data for such codes in the environment of an engineering design office, although the use of project-wide data bases and CAD/CAE systems have reduced the cycle time somewhat. Manual analysis of the numerical output from a single run can often take days. Clearly, the actual computation time for the computer runs is small compared to the elapsed time of the total engineering task at hand. The bottleneck is not usually the computer; it is the engineer/scientist. It is stark testimony to the achievements of the last 20 years that a very wide scope of problems can be routinely handled by industrial codes. There remains, of course, no shortage of critical problems that remain (such as the lack of experimental data for extreme accident scenarios) but these lie outside the domain of simulation proper. However, I hope to illustrate that simulation will play a key role in pushing out the boundaries of our experiments and theories.

Since I have little direct experience with Computational Fluid Dynamics (CFD), my comments shall have to be brief. Some 12 years ago I had the pleasure of hearing Pat Roache give a paper on CFD. His work [ROA76] codified the notion that CFD had gained the status of being a compliment to wind tunnel experiments. The effects of many different designs over a wide variety of precisely controlled boundary and initial conditions could be tested computationally many times faster, more cheaply and with comparable accuracy than could be done experimentally, say in a wind tunnel. A recent presentation by NASA at a CFD workshop [GRA88] echoed the same sentiment. In one situation, simulations were used to diagnose a faulty wind tunnel probe placement. Further, the art of simulation (and hardware development) now permits the modeller to don a helmet containing stereo vision screens which effect 3-D simulation graphic output that is keyed to the modellers position. The modeller can literally walk around a simulated aircraft and view the streamlines calculated by the code. Simulation models also allow a form of inverse design: specific terms in the governing equations can be monitored and their values correlated to the results. A new era of simulation is upon us! There is a distinct qualitative difference in such simulation tools over the calculations of the past.

The nuclear and chemical process industries also have made distinct qualitative gains. CAD/CAE systems perform 3-D renditions of plant layouts and permit the user to 'walk around' the plant, check lighting, interferences, etc. The adage, Garbage In / Garbage Out, should now be replaced by Graphics In / Graphics Out. After all, humans are primarily pattern recognition machines. We never have been or will be good at number crunching. It behooves us to interact with machines on OUR terms if we are to make the most of the ART of science.

Having given away my punchline, let us develop the theme more systematically.

THE QUEST: From Simulation to Stimulation

To advance the art of science, I offer a modest proposal. First, is the enhancement of the current endeavours by the reduction of the perspiration and tedium involved in simulation. Herein I note the pedristrian idea of code sharing, I offer some thoughts on code generalization, and I outline a new growth path for simulation involving artificial intelligence (AI). All these offer the chance to enhance simulation and reduce the time spent on low level activities. This will leave more time for inspiration. I also discuss vehicles currently underway at McMaster University that may ultimately enhance that process directly. First, the reduction of perspiration.

- Enhancements to the Rational Process: Code Sharing

We all have many common routines that others would find useful. Some of these routines are quite specific. These could be made generally available through a clearing house, but I think their usefulness would be limited to existing user groups for that application. We should target those routines which are general and are commonly useful, such as material property routines, numerical algorithms, etc. Much is already available via TOMS, EISPACK, LSODE, etc. for numerics, but general routines tuned for the simulator must come from the simulationist, not the numerical analyst. Many simulation specific subroutines are available within specific industries or clusters of industries, but are not generally available. We must open the doors to all. How many times do we need to re-develop water property routines before we cry "ENOUGH"? At this and subsequent conferences we have the forum for software exchange. We only have to use the opportunity we have in front of us. I suggest we merely have to announce the availability of a routine or package by supplying the conference organizer with a one page summary, with address, cost, etc. This summary could be bound with the proceedings. We could also make our needs known in a similar way. To start the ball rolling, I offer H_2O properties [GAR88,89a], as per Appendix I.

- Enhancements to the Rational Process: Generic Thermalhydraulic Models

Further to the enhancement of current simulation by the reduction of perspiration, we need to step back and look at simulation as an element in a larger project. Much is usually made of the enhancement of a simulator by the discovery of a faster algorithm. Obtaining a speedup of a factor of 2 is a notable event worthy of praise. But is it needed? Where is the bottleneck in your project environment? For the nuclear industry, the elapsed time for project completion, from project concept to inservice, is not significantly affected by simulation run time. Rather, the engineering phase is governed by concept generation, data preparation, model definition, coding, debugging, code verification, analysis, and design. A slow running code that is easy to use, modify or develop, even though it is not the last word in accuracy, is a clear winner over the exotic, temperamental, accurate and speedy A-stable, implicit, ASAD (all singing-all dancing) code.

But, alas, the real world demands compromises, a balance must be sought. Some enhancements over a naive explicit number cruncher are essential for stiff systems (for instance) and well worth the price in coding. The key thing to note, however, is that the parameter to optimize is not speed of computation, or stability or robustness per se. We need to optimize the overall project, not the code. In this regard, the optimum code is one that gets the job done with the minimum of fuss and muss. Keep in mind, however, that some careful planning in code design

can lead to big payoffs down the line. For instance, effort spent in modularizing a code or generalizing it so that the code serves more than one project is often well spent. The ART is knowing when to stop modularizing and generalizing. Our experience has shown, for instance with the KEE[3] operating environment on the EXPLORER[4] LISP machine, that small jobs can be more efficiently done in C because more time was spent turning off the bells and whistles of KEE than was spent programming directly in C.

To offer a concrete example, let us look at the simulation of a thermalhydraulic loop of a CANDU reactor and some of the scope for variations with a view to embodying a spectrum of situations into one code. The primary equations are the conservation equations for mass, momentum and enthalpy. In general, we have:

$$\iiint \dot{\psi} d\tau + \iint \psi v \cdot ds = \iiint \Gamma \, d\tau + \iint S \cdot ds \tag{1}$$

where ψ = field variable, ρ, ρv or ρh
- v = velocity
- S = surface source or sink
- Γ = volume source or sink
- ds = elemental surface area
- $d\tau$ = elemental volume
- ρ = density
- h = enthalpy
- t = time.

This equation is not directly solvable and so, immediately, some assumption is required to make it tractable. When modelling detailed flows (in 1, 2 or 3-D), we usually apply Gauss' theorem:

$$\iint \psi v \cdot ds = \iiint \nabla \cdot \psi v \, d\tau \tag{2}$$

(Which only strictly applies for continuous fields.... and is not true over phase boundaries). Applying the theorem and dropping the volume integrals we find

$$\dot{\psi} + \nabla \cdot \psi v = \Gamma + \nabla \cdot S \tag{3}$$

and we get the usual mass, energy and momentum eqns:

$$\dot{\rho} + \nabla \cdot \rho v = 0 \tag{4}$$

$$(\dot{\rho v}) + \nabla \cdot \rho v v = -\nabla P + \nabla \cdot \tau + \rho f \tag{5}$$

$$(\dot{\rho h}) + \nabla \cdot \rho h v = -\nabla \cdot q + Q + \tau : \nabla v + \dot{P} + v \cdot \nabla P \tag{6}$$

This form of the basic equations are usually used for problems involving detailed flows in tanks, pipes, etc. Note that the momentum equation introduces a new parameter: pressure, P.

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[3] KEE, Knowledge Engineering Environment, is a Trade Mark of Intellicorp.

[4] Explorer is a Trade Mark of Texas Instruments, Inc.

For friction dominated flows, we can specify a boundary pressure at some point in space and march out the solution to this parabolic problem. Even for the single phase case, there are many traps awaiting the unwary modeller: numerical diffusion (artificial viscosity), mass loss if you use the non-conservative form, numeric instabilities, not to mention excessive memory requirements and run times for 2 and 3-D problems.

For problems that are not dominated by friction, such as boiling, natural convection, etc., the equation of state (EOS) must be introduced to obtain closure: $P = P(\rho,h)$. This adds a time consuming complication. Add to this the possibility of non-equilibrium two-phase flow with different phase velocities and you are forced to consider 6 conservation equations and 2 equations of state plus empirical correlations for interphase mass, momentum and energy transfer (which are still quite uncertain).

Consider again equation 1, but this time, let us focus on surface fluxes for the purpose of modelling the heat transport system of a nuclear reactor as a hydraulic network of pipes. This network can be represented by a series of nodes joined by links (figure 4). Changes in mass, pressure and enthaply occur at the nodes. Momentum changes occur in the links. Thus the network is treated on a macroscopic scale, requiring an integral representation of the fundamental equations.

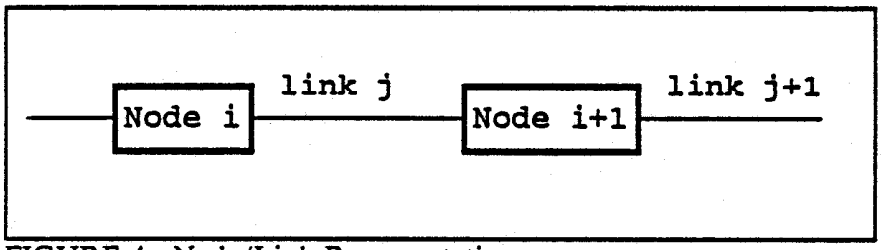

FIGURE 4. Node/Link Representation

The surface integral representing mass convection through the node, can be written as surface integrals over the individual flow paths into and out of the volume or node. That is,

$$-\int\int \rho \mathbf{v}\cdot d\mathbf{s} = \sum \rho_{in} v_{in} A_{in} - \sum \rho_{out} v_{out} A_{out} \qquad (7)$$

where A is the flow cross sectional area for the inflows and the outflows. Velocity and density are assumed to have uniform profiles across the face of each link, representing average values for the pipe. Thus we now have:

$$\dot{M}_i = \sum \rho_{in} V_{in} A_{in} - \sum \rho_{out} V_{out} A_{out} \qquad (8)$$

where $W = \rho v A$ = the mass flow through the link and M is the total mass in the node. The momentum equation becomes:

$$\dot{W}_j = (A_j/L_j)\,[P_{ie}-P_{ix}] - K_j\,|W_j|\,W_j - b_{wj} \qquad (9)$$

where L is the link length, ie and ix are the entrance and exit nodes, respectively, of the link, K is a constant of resistance and b_w is a catch-all term covering body forces. The enthalpy equation becomes:

$$\dot{H}_i = \sum W_{in} h_{in} - \sum W_{out} h_{out} + b_{hi} \qquad (10)$$

where H is the total enthalpy of the node, heat flux and generation terms have been lumped into a heat source, b_{hi}, and minor terms are dropped.

This is the lumped or macroscopic form often used in process plant simulation. The bulk of the industry standard nuclear plant simulation codes utilize this form. As for the microscopic form, many variations abound, depending on number of phases, degree of non-equilibrium, etc. The microscopic and macroscopic forms are simply different views of the same phenomena. Once focuses on gradients, the other on surface fluxes.

The above situations have been studied with great energy and genius over the last 30 years and codes abound for many diverse situations. The solution techniques for the two classes, micro vs macro, diverge from the outset and little common ground exists. How can one possibly conceive of code unification and a rationalization on the practical working level of the simulationist?

I certainly do not possess the holy grail of the grand unifying solution, but my work with the macroscopic form [GAR87a,b] has permitted me to make the following insight. The describing system equations for thermalhydraulic equations must contain all the important characteristics and, thus, one must consider the fundamental nature of the basic equations. One must address the mathematical analogue of the physical flow. This analogue is the flow of information. Illustrated in figure 5 are the equations and the information links between them. In words, the momentum equation gives the flows or velocities from one node to another, or from one grid point to another, based on the local pressure, mass amd enthalpy. The updated flows are used by the mass and enthalpy equations to update the mass and enthalpy content at each location. This information is given to the equation of state to update the pressure distribution. This pressure, along with the new densities and enthalpies are used by the momentum equation, and so on. In this manner, a time history of the fluid evolution is obtained. Thus the equation of state is one of the four cornerstones in the flow of information in single and two-phase flow. The equation of state, $P = P(\rho,h)$ can be recast

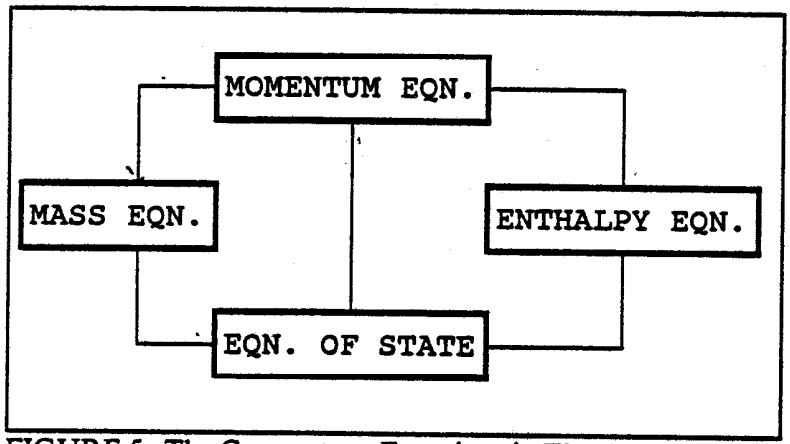

FIGURE 5. The Cornerstone Equations in Thermalhydraulics

$$\dot{P}_i = G_{1i}\dot{\rho}_i + G_{2i}\dot{h}_i = C_{1i}\dot{M}_i + C_{2i}\dot{H}_i + C_{3i}\dot{r}_i \qquad (11)$$

where G_1, G_2, C_1, C_2 and C_3 are slowly varying functions of P [GAR87b]. This puts the EOS on the same level as the conservation equations: as rate equations. Previously, the EOS was relegated to the role of a correlation. Now, it is a full partner in thermalhydraulic flow. This is important since the dominant parameters in loop flow are the flow and the pressure, (as per the classic spring-mass problem).

For the fully-implicit method, the conservation equations of mass, momentum and enthalpy must be cast in implicit form (herein, the notion of a switch, S, is used to permit a user controlled variation in the degree of implicitness from fully explicit when S=0, to all when S=1):

$$\dot{M}_i = \Delta M_i/\Delta t = \sum_{in} (W + S_{MW}\Delta W) - \sum_{out} (W + S_{MW}\Delta W) \tag{12}$$

$$\dot{W}_j = \Delta W_j/\Delta t = (A_j/L_j)[P_{ie}+S_{WP}\Delta P_{ie} - P_{ix}-S_{WP}\Delta P_{ix}]$$

$$- K_j |W_j| W_j - 2 K_j S_{WW} |W_j| \Delta W_j + b_{wj} \tag{13}$$

$$\dot{H}_i = \Delta H_j/\Delta t = \sum_{in} (W_k+S_{HW}\Delta W_k)(H_k+S_{HH}\Delta H_k)/(M_k+S_{HM}\Delta M_k)$$

$$- \sum_{out}(W_k+S_{HW}\Delta W_k)(H_k+S_{HH}\Delta H_k)/(M_k+S_{HM}\Delta M_k) + b_{hi}$$

$$= \sum_{in} (H_k/M_k)(W_k+S_{HW}\Delta W_k) + \sum_{in} (S_{HH}\Delta H_k/M_k)W_k - \sum_{in} (S_{HM}H_k\Delta M_k)W_k/M^2_k$$

$$- \sum_{out} (H_k/M_k)(W_k+S_{HW}\Delta W_k) - \sum_{out} (S_{HH}\Delta H_k/M_k)W_k + \sum_{out} (S_{HM}H_k\Delta M_k)W_k/M^2_k + b_{hi} \tag{14}$$

The overall procedure is to substitute equation 12 into equation 14 to eliminate ΔM and obtain ΔH in terms of ΔW (this will involve a matrix inversion). Then we substitute equations 12 and 14 into equation 11 to yield ΔP as a function of ΔW. Substituting this result into the momentum equation gives a single equation in ΔW. This is the fully implicit, back substituted form. In matrix notation:

$$\dot{M} = A^{MW}W^t + S_{MW}A^{MW}\Delta W \tag{15}$$

$$\dot{W} = A^{WP}(P + S_{WP}\Delta P) + A^{WW}W^t + 2\, S_{WW}A^{WW}\Delta W + B_W \tag{16}$$

$$\dot{H} = A^{HW}W^t + S_{HW}A^{HW}\Delta W + S_{HH}A^{HH}\Delta H - S_{HM}A^{HM}\Delta M + B_H \tag{17}$$

Rearranging for $\dot{H}$ in terms of W and ΔW,

$$\dot{H} = [I - \Delta t S_{HH}A^{HH}]^{-1}[A^{HW}(W^t + S_{HW}\Delta W) - \Delta t S_{HM}A^{HM}A^{MW}(W^t + S_{MW}\Delta W) + B_H] \tag{18}$$

For fixed volumes, equation 11 in matrix notation is expressed as

$$\dot{P} = C_1 \dot{M} + C_2 \dot{H} \tag{19}$$

The mass and enthalpy equations can be substituted into equation 11 to cast $\dot{P}$ as a function of flow:

$$\dot{P} = C_1A^{MW}(W^t + S_{MW}\Delta W) + C_2[I - \Delta t S_{HH}A^{HH}]^{-1}[A^{HW} - \Delta t S_{HM}A^{HM}A^{MW})(W^t + S_{HW}\Delta W) + B_H] \tag{20}$$

$$= A^{PW1}W^t + A^{PW2}\Delta W + B_P$$

This is substituted into the flow equation to give:

$$[I - 2\Delta t S_{WW}A^{WW} - \Delta t^2 S_{WP}A^{WP}A^{PW2}]\Delta W =$$
$$\Delta t\{[A^{WW} + \Delta t S_{WP}A^{WP}A^{PW1}]W^t + B_W + \Delta t S_{WP}A^{WP}B_P + A^{WP}P\} \tag{21}$$

which is of the form A x = b. After solving equation 21 for the new flows, the masses and enthalpies and pressures are updated using equations 15, 18 and 19, respectively.

This form was found to be quite robust and stable. Subsets of this form are found in the now classic work of Porsching[POR71] (where $S_{HH} = 0$ and all other switches = 1). RETRAN's scheme is evolving from Porsching's scheme towards this fully implicit scheme. Variations exist in the method used to solve the final matrix equation A x = b.

The form presented here deliberately carries the switches through to the end so that the user can try variations on a theme to tailor the scheme for his or her situation. For instance, if small timesteps are required anyway due to some outside constraint, there is no need to incur the extra expense of the implicit formulation. Therefore, all switches can be set to 0 to achieve the fully explicit method. If time steps are restricted to the Courant limit, then the semi-implicit method (as per Porsching) is sufficient. The method is thus very general and encompasses a wide class of process simulation needs.

On another level, we gain insight and unification by considering the microscopic form of the momentum equation:

$$(\dot{\rho v}) + \nabla\cdot\rho vv = -\nabla P + \nabla\cdot\tau + \rho f \quad . \tag{5}$$

and noting that we can write the future value of pressure as:

$$P^{t+\Delta t} = P^t + \Delta t\dot{P} \tag{22}$$

we find (after some manipulation):

$$(\dot{\rho v}) + \nabla\cdot\rho vv = -\nabla P^t + \Delta t G_1 \nabla^2 \rho v + \nabla\cdot\tau + \rho f$$

$$+ \Delta t G_2 \nabla[1/(\rho - G_2)(\rho\nabla\cdot hv + \nabla\cdot q - Q - \tau:\nabla v - v\cdot\nabla P + G_1\nabla\cdot\rho v)] \tag{23}$$

Thus the equation set of 3 conservation equations plus the EOS for each point in space is reduced to a single momentum equation for each point in space which should be well behaved numerically since it is diffusive in nature. Implicit formulations are now much reduced in size and hence are much more tractable. Initial work indicates this approach leads to stable, fast and robust solutions.

In short, I find that organizing with respect to information flow has led to a focus on the flow and pressure equations as the dominant equations in power loops. Casting pressure in the form of a rate equation causes a change in focus that is instructive and practical for numerical solutions. It leads to a general, efficient scheme which would be of use in reducing the tedium in simulation.

The above constitutes my modest attempt to reduce the perspiration by making a small step toward unifying the copious solution techniques for thermalhydraulics.

- Enhancements to the Rational Process: Artifical Intelligence (extracted from [GAR89b])

Another attempt at simulation enhancement is the marriage of numeric and symbolic computation such as the work underway at McMaster. The concept is modular, robust and has a clear upward growth path. Work is proceeding with the reduction of perspiration in mind. Herein, we investigate the integration of symbolic computation and reasoning into highly computerized numerically-based real-time control systems for complex plant process management. The particular implementation involves nuclear power plant intelligent monitoring and the development of suitable subsystems that are required for the Operator Companion as shown in figures 1 & 3 of [GAR89b], reproduced here as figures 6 & 7.

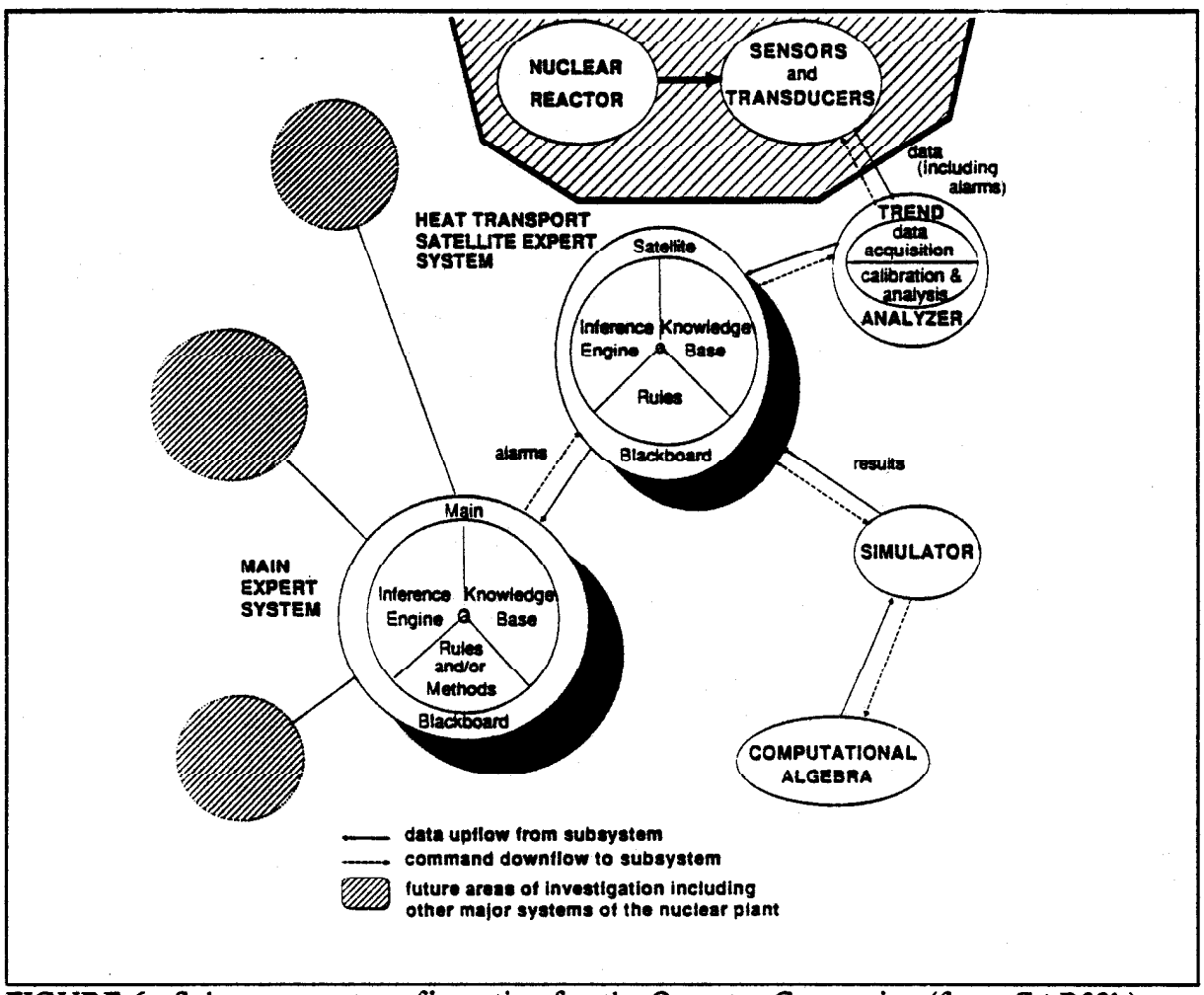

FIGURE 6. Subcomponent configuration for the Operator Companion (from GAR89b)

The Operator Companion is a knowledge-based system that can assist the operator of a nuclear (or conventional) power plant to diagnose faults and abnormal conditions and to respond to them in an appropriate manner. An expert system is needed here because a nuclear power plant with its many components can fail in a large number of ways, each of which may give rise to a variety of alarm signals. The resulting complexity of the alarm display can easily produce a state of information overload in the operator [SPE87]. The analytic or reasoning capability of the expert system can be brought to bear on the problem of condensing the large number of outputs into a few easily comprehensible signals. This is a good example of sensor fusion, the reduction of a collection of measured data to a single synthetic variable which represents the current state of a complex system [LEC86]. Thus, the design and implementation of an Alarm Pattern Analyzer is central to the development of any operator companion and forms part of

the main expert system. Intelligent alarm recognition provides the operator with a basic tool to determine the class of events that could give rise to an observable alarm pattern.

The central control strategy has an expert system as the system master. This master utilizes high level information provided by satellite processors (involved in data acquisition, trend analysis and simulation). These subprocessors can be symbolic or numeric in nature as required. Off-loading the master processor via the subprocessor configuration can potentially resolve many problems imposed by real-time performance and provide the high level arbitration capability needed. However, the resulting distributed systems now require that significant attention be paid to a suitable communication strategy to be effective.

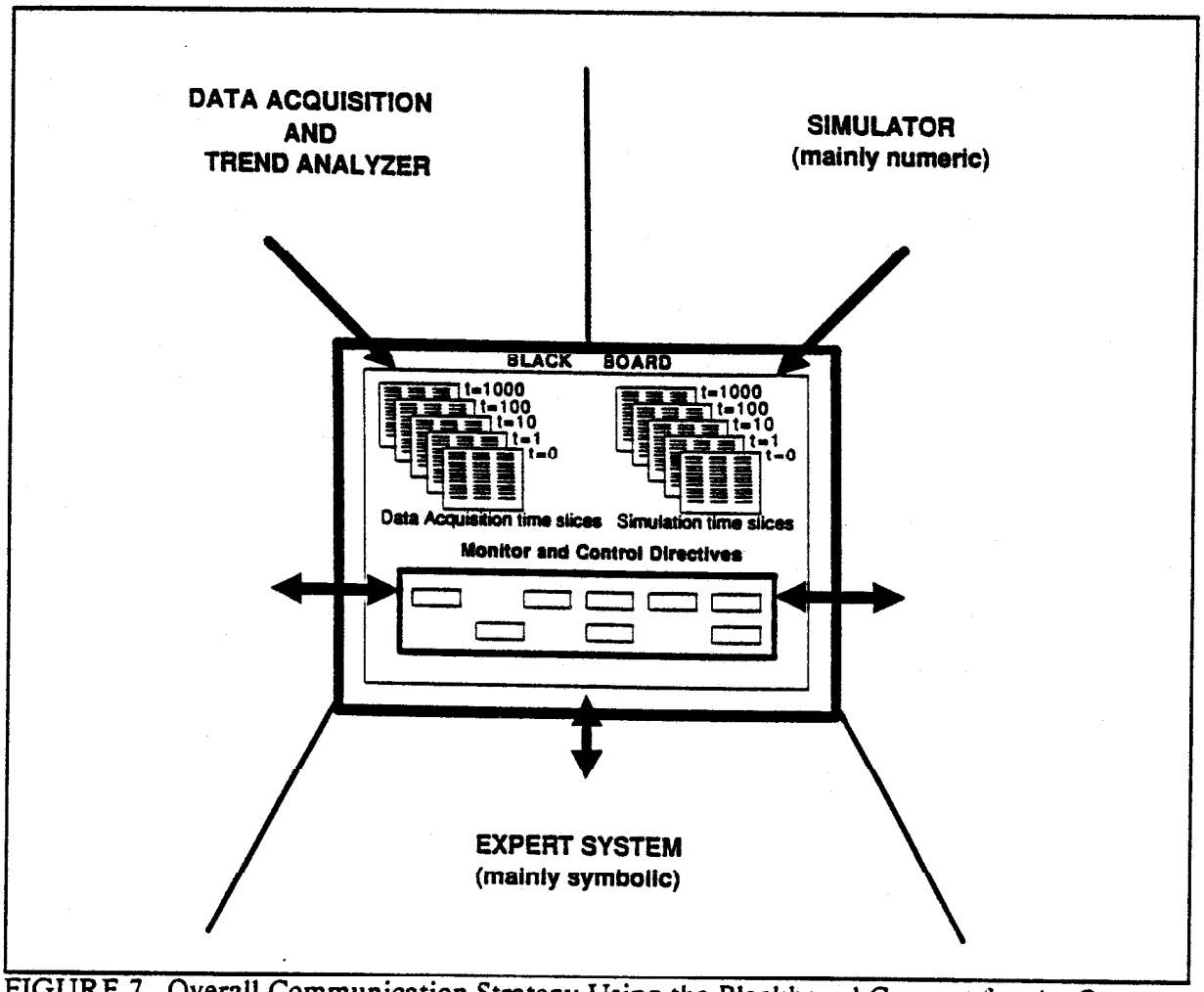

FIGURE 7. Overall Communication Strategy Using the Blackboard Concept for the Operator Companion (from GAR89b)

The blackboard concept [ERM80,NII82] plays a major role in providing the required functionality in communication and the blackboard itself is amenable to implementation on a separate processing engine [LEV87] (see figure 7, taken from [GAR89b]). Although utilized primarily as a global structure to promote cooperative problem solving amongst a group of independent knowledge sources, this strategy is useful for both numeric and symbolic information passing. As with the original implementation [BAR81], it provides advantages of modularity and flexibility where the restructuring of the system is easily accomplished while allowing various control strategies to be explored.

The trend analyzer observes trends typically on the order of seconds, minutes, hours or even

months. This allows the identification of problems of high frequency through to slow deterioration. To detect deviation, a baseline is, of course, necessary. Hence, the trend analyzer consists of a data storage section (time slice snapshots) and a generic numeric/symbolic calculation section for computing expected values, setting indicator flags, etc.

An important operation for a human expert is the use of mathematical expressions for the description of the operating conditions in an engineering system. Computer algebra systems exist for the manipulation of symbolic expressions used in modeling systems in structural mechanics, high energy physics, and quantum mechanics. Research over the past decade has aimed at improving algebraic algorithms and building faster and more portable systems [ZIP84]. A system, such as that envisaged by Zippel, should help the user to derive the differential equations needed to describe, for example, the mass, momentum, and energy transport equations for coolant flow in a nuclear reactor. This tool allows the user to derive and simplify the transport equations in the desired reference frame and coordinate system (Cartesian, cylindrical, spherical). Thus, the user can interactively transform the equations as needed and display them typographically, i.e., by means of a suitable mathematically correct character font.

The work described in [GAR86] has resulted in an interactive program, EQNWRITE, which permits the following manipulations of the transport equations characteristic of thermalhydraulic work: (1) switching between Euler and Lagrange coordinate frames, (2) switching between volume and surface integrals, (3) grouping together of terms and factors, (4) user directed simplification, and (5) the application of differential and integral calculus procedures. The program was developed on a personal computer with the help of the MUMATH, a microcomputer-based symbolic mathematics system [SOF83].

Symbolic mathematics systems can be considered as an aid to the system expert, as well as the operator, in the form of a tool for back-of-the envelope symbolic calculations. They can also be of value in prototyping simulator subsystems through the automatic generation of source code directly from the algebraic equations.

The final component of the satellite system is a simulator. It consists of two portions. The first portion performs calculations specific to small loss of coolant accident (LOCA) analysis. These would include calculations of mass inventory and rate of leakage, estimation of water storage tank drainage time and reactor trip time, overall heat balance and any other pertinent calculations. The second part is a simulation of the heat transport system as described in the previous section.

Note that intelligence in the form of rules must be coded into the trend analyzer, blackboard and Expert System. Bearing in mind that the Heat Transport System is but one of dozens of key plant systems, we are left with a major coding task for each new station since even the so-called 'repeat' stations have a large number of subtle changes from the preceeding designs. One notion to circumvent the laborous recoding process is the use of neural nets [VOE87]. The neural net essentially replaces the weights used as confidence factors in rule-based expert systems. But more importantly, and on a deeper level, neural nets provide a valuable link between the station inputs (trends) and the desired output (diagnosis of events). First, the significant inputs are identified (power, pressure, temperature, flows, alarms, etc.). Second, the desired events to diagnose are identified (loss of coollant, normal power, crash cooldown, etc.). The neural net (essentially a matrix of links connecting all possible inputs to all possible outputs) is 'trained' by feeding real or simulated event data to the net and algorithmically

adjusting the strength of the links (weights) until the event is recognized (i.e, the output is a signal denoting the event). No rules are coded! For a new station, the plant simulator (which must be built anyway) is plugged into the neural net and the net is retrained, automatically accounting for subtle differences between stations.

Alas, all of the above, even the AI work (with the exception of the neuralnets), are strictly rational processes. They do not address the non-rational (perhaps this is why AI is not Real Intelligence). So far, we have discussed the reduction of perspiration for the purpose of freeing up our minds to the task of inspiration. So, let us move on to our real QUEST, the stimulation of inspiration.

- Enhancements to the Non-Rational Process: The QUEST for the Holy Grail

The type of working environment that a scientist or engineer seeks can perhaps be better described by analogy to creative writing. Imagine a word processing machine that has a 10 minute delay between the time a key is pressed and the time a letter appears on the screen. The writer certainly would find that the process of creative writing to be severely curtailed. The human mind thrives best when there is a rythme or flow of ideas, with fast, continuous feedback and interaction. Typically, the scientist/engineer must endure lengthy time delays in most aspects of simulation, from concept to coding, through to debugging, verification, running and analysis. No where and at no time do these time delays lead to more sterility than in the concept phase.

Our QUEST then is the creation of an environment that permits the easy exploration of ideas. For illustration, consider the task of thermalhydraulic simulation. In scoping out a new process loop design, back of the envelope calculations are usually too crude and full scale simulations are too cumbersome, expensive and time consuming to be warrented. Yet, scoping studies must be done, managers must be convinced, untenable ideas must be weeded out. Further, one should be able to tap into existing databases to make good use of existing knowledge pools. And, presumably, any progress made in the scoping stage should contribute back to the knowledge pool. Better still, there should be a seamless, upward growth path for code development, including input and output data sets.

There typically is a wide variety of needs in scoping studies. Steady state and transient solutions are needed, as are system eigenvalues or stability maps. The focus or scale can switch from a myopic view of a valve to the overall view of the behaviour of the system. We need to be assured that our modelling is approximate yet not crude. Our scoping tools must be robust enough to withstand abuse, failing gracefully, not catastrophically. Of course, the code must be 'user friendly' in the front and rear end.

This indeed is a holy grail! No computer code exists that can supply these things. Yet some inroads have been achieved. At McMaster, work is underway on a microcomputer based code, illustrated in figure 8, called THEME (Thermalhydraulic Engineering Modelling Environment). The input section is similar to a CAD or object based drawing package. Predefined objects, such as pumps, valves, pipes, vessels, etc, are selected at will and a process loop is rapidly constructed on the screen. As the schematic is being drawn, data links are created in the background and the skeleton of the input data file is formed. The user can fill in process information (such as volumes, lengths, etc.) as it becomes available. The input structure mimics that of a standard industry mainframe code so that the THEME can be used as a front end for

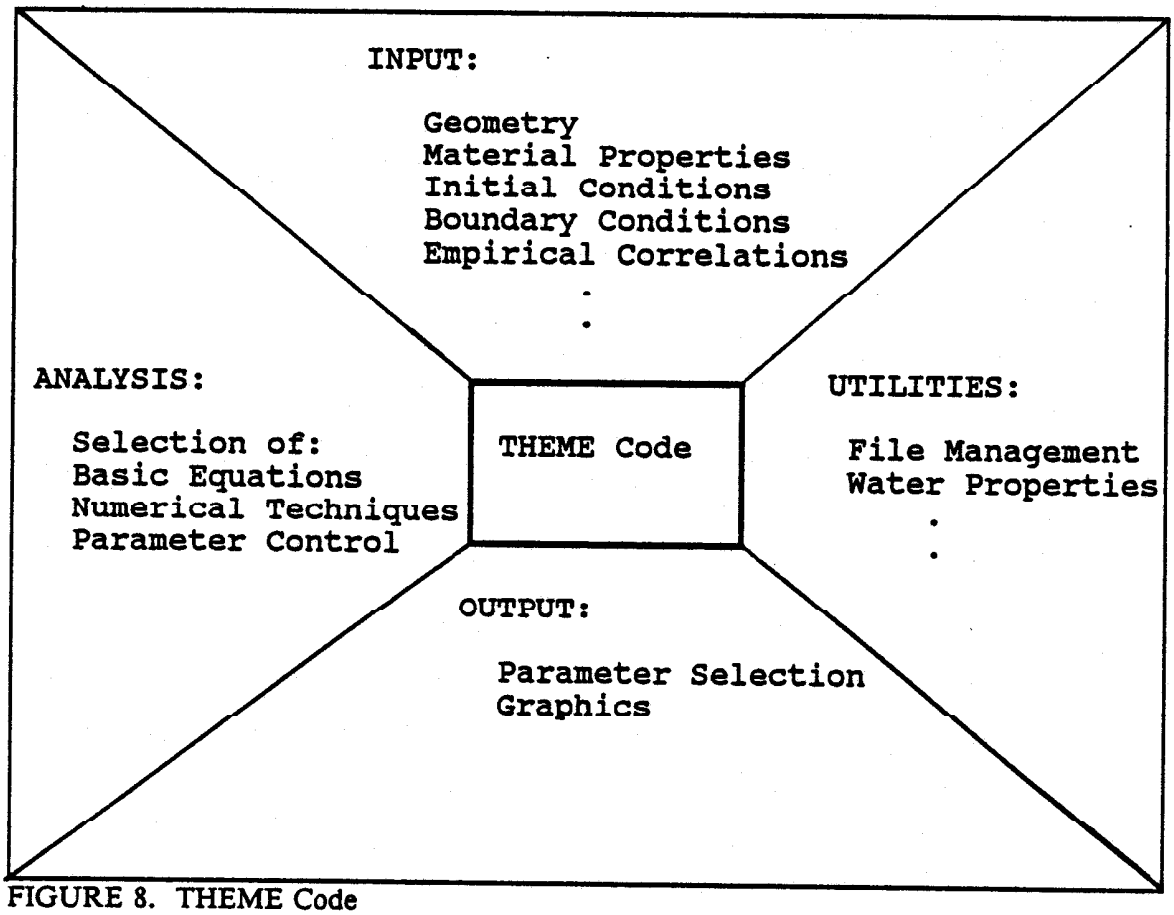

FIGURE 8. THEME Code

the mainframe code, as well as a self-contained microcomputer based simulation code. The upward migration path is thus ensured and as a bonus, the same data file can be used to run both the scoping tool and the mainframe code, providing an extra degree of verification.

Moving from the input creation phase to the analysis phase, the user selects the type of analysis to be performed and perhaps decides whether to over-ride default settings for the switches in numerical methods. The simulation is invoked and OUTPUT section parameters control the storage and presentation of output. The UTILITIES section is the catch-all for miscellaneous items such as a temporary exit to the operating system, invoking editors, pop up calculators and selecting subprograms such as steam tables, empirical correlations, etc., whose results may be cut and pasted into the input section if required.

Although development is still in the early phase, we have shown that the concepts are doable. All the basic concepts have been implemented on a PC to show their feasibility.

Another implementation with much the same QUEST is the G2[5] code of Gensym Corporation. This implementation is a workstation based real-time expert system LISP code of very impressive proportions that is commercially available today. It is intended primarily for real-time process diagnosis. Rather complete process schematics can be built in a few hours with hooks to existing procedures in C and FORTRAN simulation code that you might already have. Although you will inevitably come up against the constraints of a closed system (such as limits

[5]G2 is a trademark of Gensym Corporation

to time step control that might fall just short of your desires on algorithm control), the capabilities of this code are so large that meaningful scoping studies should be well within your grasp. This tool appears to be a superb vehicle for intuition generation.

Of course, we should not overlook the entirely new gendre of scoping tool embodied in the spreadsheet. Who hasn't used one to quickly correlate some data, quickly plot up some output results from a FORTRAN code, or visualize a correlation. An a $75 addin to my spreadsheet allows me to plot the results in 3 dimensions at the press of a few keystrokes. One could also use spreadsheets for preparing formatted input to an existing simulation code. I have a rather simple worksheet for calculating a heat balance of a CANDU power plant that was done as a student example [GAR85]. It is now being used by an electrical utility, not because it is brilliant, but simply because it is handy. With it, the design engineer can quickly see the effect on power calculations if, for instance, one of the flow instruments should fail. By spending 1/2 hour with this spreadsheet, the designer can get a good grasp of the bulk effect of many design decisions. The spreadsheet is an excellent intuition stimulator.

CONCLUSION

From our brief examination of the role of simulation in science and engineering endeavours, it is evident that simulation has grown from the role of extended calculator to that of inspiration stimulator. Simulation is firmly entrenched in the scientific method. Work needs to continue on algorithm generalization so as to free up head space for the more important tools of intuitive generation and discovery. It is also evident that today's simulation tools, even at the low end, offer much to the user in terms of the exploration of non-rational processes.

ACKNOWLEDGEMENTS

The McMaster work referenced herein involved the contributions of students and colleagues over the last 5 years. Special thanks are given to Skip Poehlman, Nick Solntseff, Bob Wilson, Betty Moll, Rayman Sollychin, John Hoskins and Brian Hand for their hard work and stimulating conversations.

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NOMENCLATURE

A	flow area (m^2)
A	general system matrix
b	constant
B	constant vector
f	body force
$G_1,G_2,C_1..C_3$	thermodynamic coefficients
h	specific enthalpy (kJ/kg)
H	total enthalpy (kJ)
I	identity matrix
K	resistance coefficient
L	length (m)
M	total mass (kg)
P	pressure (Pa)
Q	heat source/sink
q	heat flux
S	switch
S	general surface sink or source
s	surface vector
t	time (s)
τ	volume (m^3)
v	velocity vector
W	mass flow (kg/s)
x	general vector
ρ	density (kg/m^3)
ψ	general field variable
Γ	general volume sink or source

SUBSCRIPTS /SUPERSCRIPTS

e	entrance
i,j,k	link or node indices
in	inlet
out	outlet
x	exit
H	reference to enthalpy
M	reference to mass
P	reference to pressure
W	reference to flow

OPERATORS

$dx/dt = \dot{x}$	time derivative
∇	del
Δ	delta (difference)

ACRONYMS

AI	Artificial Intelligence
CANDU	Canadian Deuterium Uranium
CFD	Computational Fluid Dynamics
EOS	Equation of State
HTS	Heat Transport System
LOCA	Loss of Coolant Accident
QUEST	Quintessential Eureka Stimulator

APPENDIX I

ITEM: H_2O property fits

LANGUAGE: FORTRAN 77

Transfer MEDIA: One 5 1/4" Floppy Diskette - IBM PC format. 360 Kb ASCII text files (MS-DOS).

MACHINES: Designed for IBM and compatible microcomputers, portable to most FORTRAN compilers since no exotic programming is used.

SOURCE CODE SUPPLIED: YES

DESCRIPTION: Low order polynomial curve fits were obtained based on the 1984 NRC/NBS steam tables. These fits are fast and accurate, and cover subcooled, saturated and superheated H_2O over the pressure range 0.7 MPa to 22 MPa and the temperature range 80°C to 450°C. Accuracy for commonly used properties are usually of the order of 0.1%.

LIMITATIONS:

COST: $50 to cover postage and handling is requested, but is not obligatory.

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