Working Group on Hybridization between R&S, DoE and Optimization

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This is the report of the working group on the relation between, or hybrid combination of design experiment optimization and R&S. The rapporteur, Paul Kantor, learned a great deal at the conference which he summarized by sharing the cartoon shown here.("A student asking the teacher '...may i be excused, my brain is full' " (from a 1986 cartoon by Gary Larson)- omitted here for copyright reasons)

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Sampling-based Optimization in the Presence of Uncertainty
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Will it rain tomorrow?

- Forecasting
  - how much
  - when
  - where - will *your* plane fly tomorrow
- what makes a forecast “good”
  - mean square error *-estimation*
  - picnics ruined *-decision*
  - overflowing storage tanks *-long range decision*

We take as a simple example the issue of forecasting, such as forecasting whether it will rain. A key question is: what is it that makes a forecast “good”? Various measures include the Mean Square error of prediction, the number of picnics ruined, or long-term consequences such as overflow of storage tanks. So we found ourselves asking whether forecasting is the goal of simulation or whether forecasting a must take place in order for us to know what to simulate.

We could not give precedence to either of the two activities and found ourselves in a situation characterized by this beautiful design of two snakes, each eating the other's tail.

▫

Observations

- Simulation optimization can be viewed as sequential DoE.
- DoE is also an optimization problem, e.g., Pareto frontier of performance vs. resource.
- .

In some sense, doing an optimal simulation can be thought of as doing a sequential series of design of experiment exercises. On the other hand, design of experiment is an optimization problem. For example we look for Pareto frontier, in the various goals of the experiment and in relation to the resources consumed.

About Models

- Model fidelity/Difference in definitions of models:
  - Decision model, e.g., pick the best engineering design.
  - More detailed model under the chosen decision
  - underlying numerical approximation models
  - under-underlying physical models

We had some thoughts about models and about model fidelity. We saw the following uses for models. A model may be aimed at making a single decision or choice. The model may be a more detailed model, that is built after decision has been taken. Underneath that, there are numerical approximation models, and underneath all of that, in many cases of interest such as aircraft design, there are physical models which are believed to be "true".

Observations (Cont'd)

- Another role of optimization:
- distribution selection
- or parameter tuning,
- e.g., in MRI imaging.

Optimization may also play a role in the selection of the distributions that are going to be explored, as well as in parameter tuning. A particular example is the selection of the many parameters that are involved in processing an MRI image.

James Joyce….

- DoE and R&S can be our design tool.
- System Theory "solve most important problem "
- Nested problems
  - Effect of estimation/approximation propagation up to higher-level model.
  - How to select DoE and optimization method for a given problem.
  - Problem formulation depends on our toolkit.

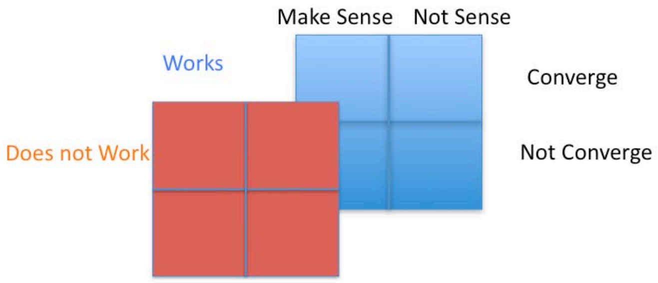
Then we have a few observations which are really stream of consciousness which is why this slide is headed by reference to the famous Irish author. Design of experiment and R&S can be a tool for design. We always have in mind the axiom of system theory, which insists that we should identify and solve our most important problem rather than one that is at hand.

We see a host of nested problems. They include asking: how the approximations made any particular level in the examination propagate up to higher levels; how to select the design of experiment model for a given problem; and finally and always, the recognition that how we formulate problems is going to depend on the toolkit that we have available for solving it.

Who cares about convergence?

- – Practical meaning of asymptotic convergence
- – Aesthetic significance /motivation of convergence results

- Three dimensions of an algorithm:



Obviously an important question in examining models is to ask about the convergence of an approximation. But we found ourselves discussing the question of "who cares about that convergence?". For example it's very common for a well-written theoretical paper to show that a result converges asymptotically. But no one ever iterates an extensive simulation to asymptote, so what is the value of this result? Is it more a question of the aesthetic motivation or a practical consideration? We found ourselves considering a threefold classification of algorithms. An algorithm that might work (the blue square) or not work (the red square). An algorithm might be proven to converge or it might not converge (this includes things that might converge without our knowing it and things that are known to not converge). Finally, and perhaps most important of all, an algorithm may even make sense or not make sense.

Fill in the blanks

- Works
  - provable
    - sensible
    - not
  - not provable
    - sensible
    - not
- Does Not Work
  - provable
    - sensible
    - not
  - not provable
    - sensible

As you can see this generates a lot of different alternatives (8) and we were able to gin up situations in which all but one of them might be of interest. We found no advocates for the algorithm that doesn't converge doesn't work and doesn't make sense ☺.

Begin with Decision Problem

- Begin with decision problem
- $f(x)=E\, f(x,\omega)$ is performance measure via simulation model
- max $f(x)$: optimization model
- Use DoE to estimate the dependence of the performance on the decision variables (or control variables, or policy)
- $f(x)=E\, f(x,\omega)$

Suppose, for example we begin with the decision problem. Then we have some function which is a performance measure, calculated under a simulation model Embedded in that end is the maximization problem. But we need to use design of experiments to estimate the dependence of performance on the decision variables.

Begin with Forecasting

- Construct best model of atmosphere*
- What should the next measurement be?
- need DOE to solve it
  - big family of models
    - below that optimization again,,,,
      - design choices
        - » optimally ...

* all particles in atmosphere plus all photons from sun

On the other hand we might begin with forecasting we need to construct a really good model of the atmosphere. We know that there is a really good un-computable model takes into account all the physical players in the game. In any case given some state of knowledge, what should the next measurement be? We need design of experiment to solve it. We have a big family of models and we know that we have some optimization again, and then we have design choices; but we want to make the design choices optimally and so on.

Good reading

- DOE -- Jack`s talk; Tom`s talk
- R&S - Steve`s talk
- SimOpt - Barry`s talk

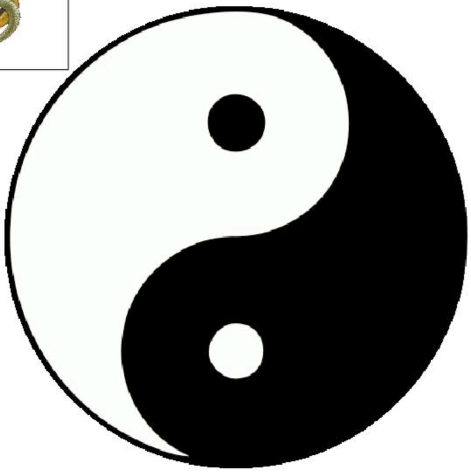
We close with some suggestion very good papers from this conference, to read on the design of experiment on R&S and on simulation and optimization

Some conclusions

- Sometimes one serves the other as subsidiary
- Usually, we enter the "problem" at some particular level, which dictates which is serving which
- Collaboration helps us understand the levels on which we are not working, by having a partner who does understand them ….*Dagstuhl MOE joint papers*.

Our conclusions are: that sometimes one serves the other as a subsidiary; that we usually enter the problem at some level in the conceptual hierarchy and that determines what we think we're serving and what we think we us as tools.

We hope that better collaboration among those of us interested in various points along the spectrum will help us to understand the levels on which we are *not* working by engaging with a partner who does understand them. And this fits very well with Dagstuhl measure of effectiveness: jointly authored papers.



"Yin and Yang are the harmony of opposites"

Rather than close with the entangled snakes, we offer finally a basic Chinese concept of the harmony of opposites. Thank you.