Optimal Design of Computer Simulation Experiments for Engineering and Architecting Systems-of-Systems Using a Main-Effects-Plus-Two-Factor-Interactions Model

Edouard Kujawski, PhD
EJK Associates
Email: edkuj@comcast.net

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Outline

- **Background**
  - Classical Design of Experiments (DOE)
  - Standard Taguchi Method (STM)
  - Optimal Design of Experiments (ODOE)
  - Huynh's Orthogonal Array Experiment (OAE)
- **Main-effects-plus-two-factor-interaction (MEPTFI) model**
- **Custom/ODOE for small boat attack (SBA) response system**
  - General approach of custom design
  - Design construction & evaluation
  - Statistical analysis
  - System allocation optimization
- **Some concluding thoughts**

Design of Experiments (DOE) What and Why

- **Definitions**

– A DOE is a structured approach to designing and analyzing experiments in which purposeful changes are made to multiple input variables (or factors) to efficiently investigate the effects on an output variable (or response).

– "A DOE is the specific collection of trials run to support a proposed model." [Donnelly, 2010]

> ➢ **ALL DESIGNS ARE MODEL DEPENDENT!**

- **Why**

– "There is not a single area of science and engineering that has not successfully employed statistically designed experiments."

[D.C. Montgomery, 2012, p. 22]

– In the last twenty years, DOE has found interesting applicability in complex industrial and military AoA that require complex computer simulations, e.g. Monte Carlo simulations.

Design of Experiments (DOE)
A Brief History (1 of 3)

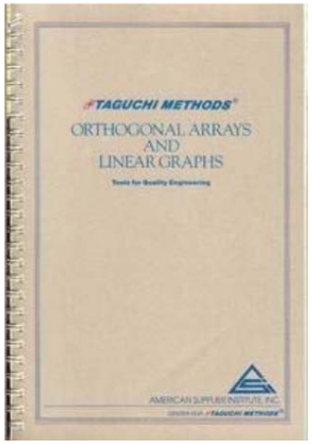
- **Classical approach, 11th – 19th centuries**
  - Vary one factor at a time
- **Foundation of DOE principles: R.A. Fisher, 1920s**
  - Full factorial designs
  - Fractional factorial designs (FFDs)
    - ☝ Reduced number of runs, e.g., 2^{k-p} FFDs
    - 👎 Confounding of main effects and interactions, i.e., biased estimates
  - Statistical analysis, ANOVA

Design of Experiments (DOE) A Brief History (2 of 3)

- **Taguchi Method, 1950s**

– *"…Robust Design* to develop industrial processes and products whose performance is minimally sensitive to factors causing variability at the lowest possible cost" [American Supply Institute]

– Small set of designs for engineers and quality professionals allowing hand calculation
  - 18 orthogonal arrays (OA)
  - Limited set of interaction matrices and linear graphs
  - Estimation of main effects by averaging appropriate response data



💣 Focus on main effects with underlying presupposition that interaction effects can be neglected

💣 Omission of statistical analysis

Design of Experiments (DOE)
A Brief History (3 of 3)

- **Optimal design of experiments (ODOE)**

– Mathematical approach proposed by Kiefer and Wolfowitz [1959]

  - DOE based on specific objective criteria rather than orthogonality
  - Does not preclude OA designs

– Recent growth in popularity

  - Custom design approach provides flexible method to design experiments that fit specific circumstance
  - Several general-purpose statistical packages, e.g. JMP,...

- **Computer simulation experiments**

– "Brute-force computation cannot be used to explore large-scale simulation experiments." [Vieira Jr. *et al.*, 2011]

– New methods being developed to more efficiently design and analyze them

  - Nearly Orthogonal Latin Hypercubes (NOLH)

Orthogonal Array Experiment (OAE) Huynh Conjectures*

** T.V Huynh, "Orthogonal array experiment in systems engineering and architecting," Systems Engineering, 14(2), 2011, pp. 208-222.*

- **Huynh's definition of OAE**
  - Synonymous with Standard Taguchi Method (STM)
  - Involves three main steps

1. Selection and reduction of Taguchi OA
2. Run experiments
3. Use of arithmetic averages of the responses for determining the effect of a factor level (STM)

- **Huynh conjectures**
  - "Application of OAEs to solve a class of engineering optimization problems encountered in systems engineering architecting"
  - "Optimum product or design results from the best or the optimum level for each factor"

The Huynh Conjectures Are False

- **Impossibility theorem**

The Huynh conjectures cannot provide meaningful results for systems and SoS engineering and architecting problems.

- **Proof**

Given: "A *system* is a combination of interacting elements organized to achieve one or more stated purposes. A *system-of-systems* is a system whose elements are themselves systems." [Haskins, 2011: 364]

Consequence: The appropriate modeling of interactions and their effects must be accounted for in the engineering and architecting of systems and SoS.

Implication: The Huynh conjectures are not applicable to the engineering and architecting of systems and SoS. **QED**

> **"Generally, when an interaction is large, the corresponding effects have little practical meaning."** Montgomery [2012, p. 186]

Main-Effects-Plus-Two-Factor-Interaction (MEPTFI) Model

"Everything should be made as simple as possible, but not simpler."

Einstein

Regression Model
Two-Factor Interaction Effects (1 of 2)

- **Pareto/sparsity-of-effects principle**

- Most real-world systems are driven by a few main effects and most high-order interactions are negligible.

- **MEPTFI surrogate model**

$$Y_u = \beta_0 + \sum_{j=1}^{k} \beta_{ju} x_{ju} + \sum_{j=1}^{k-1} \sum_{l=j+1}^{k} \beta_{ju,lu} x_{ju} x_{lu} + \varepsilon_u$$

– Y_u : response for the u^{th} run

– k factors (X_1, X_2, ..., X_k)

– x_{ju}: level-setting of factor X_j for the u^{th} run using coded design variables

– β_0: overall mean

– β_{ju}: main effect for factor X_j at the level-setting of the u^{th} run; specified as deviation from the overall mean

– $\beta_{ju,lu}$: two-factor interaction effect between factors X_j and X_l at the level settings of the u^{th} run

– ε_u: error term.

Regression Model
Two-Factor Interaction Effects (2 of 2)

- **Number of degrees of freedom (d.f.)**
  - Overall mean: 1 d.f.
  - Each factor X_i: $(n_i - 1)$ d.f., where n_i be the number of levels.
  - Each two-factor interaction $X_i{*}X_j$: $(n_i - 1)\times(n_j - 1)$ d.f.
- **Determining # distinct simulation runs**
  - Unsaturated designs: $n >$ # d.f.
  - Larger $n \Rightarrow$ higher confidence in estimates of main and interaction effects
  - Interactions significantly increase the number of required simulation runs!

Regression Model
Matrix Form

- **Model/Design matrix**

$$\boldsymbol{Y} = \boldsymbol{X\beta} + \boldsymbol{\varepsilon}$$

– $\boldsymbol{Y}$: $n\times1$ vector of the responses of the n simulation runs

– $\boldsymbol{\beta}$: $p\times1$ vector of the p unknown parameters of interest

– $\boldsymbol{\varepsilon}$: $n\times1$ vector of the errors for the n simulation runs

– $\boldsymbol{X}$: model matrix. $n\times p$ matrix consisting of an n-vector of 1s and the $n\times(p-1)$ design matrix $\boldsymbol{D}$.

– Each column of $\boldsymbol{D}$ corresponds to a factor or interaction with entries that specify the level settings. Each row specifies a design point with settings for the corresponding simulation run.

➢ Abstract representation of a general linear model (multiple linear regression model)

➢ Suitable model for DOE ranging from elementary main-effects models to factorial designs with high-order interactions

Ordinary Least-Squares Regression (OLSR)

- **OLSR estimator of vector of unknown model coefficients**

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{Y}$$

- **Variance-covariance matrix of estimator**

$$\mathrm{var}(\hat{\boldsymbol{\beta}}) = \sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1}$$

- **Fitted regression model**

$$\hat{\boldsymbol{Y}} = \boldsymbol{X}'\hat{\boldsymbol{\beta}}$$

☞ **Applicability: i.i.d. residual errors with N(0, σ^2)**

– Else use Generalized Linear Models [Montgomery, 2012, p. 645]

> **"DOE should allow DOT&E to make statements of the confidence levels we have in the results of the testing."**
>
> [DOT&E, 24 November 2009]

Custom/Optimal Design of Experimental Computer Simulations for SBA Problem

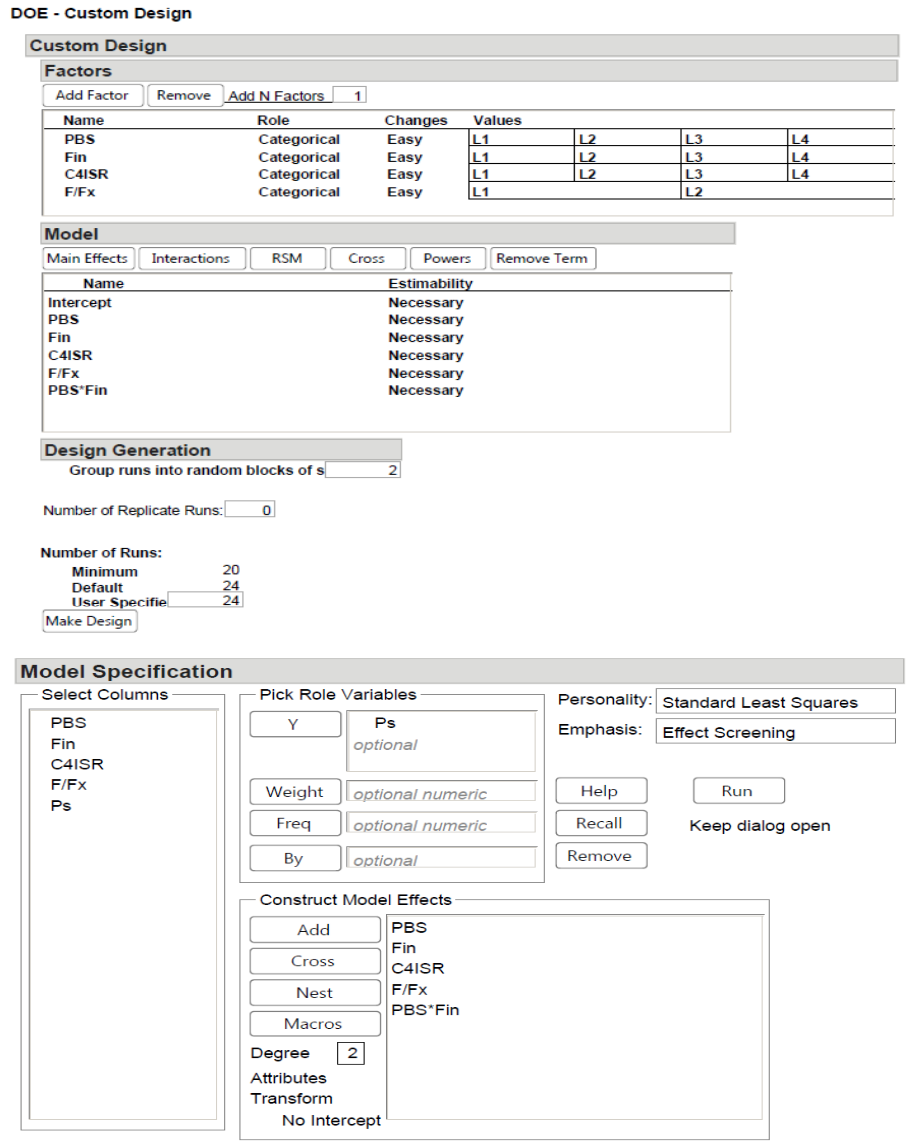
"Building experimental designs unique to the situation at hand is wonderful and profound in its importance."

J. Stuart Hunter, JMP Discovery Summit, September 2012

Custom/Optimal Design Using JMP General Approach

- **All designs are model dependent**

1. Define response and factors
2. Define model
   - Main factors, interactions, and power terms
   - Specify “Necessary” or “If Possible”
4. Specify # of runs
   - Based on # d.f. & desired CL
   - Time/cost/capability constraints
5. Specify optimality criterion
   - *D*-optimal designs most appropriate for screening experiments
6. Make design
7. Check/Evaluate design
8. Run experiments or simulations
8. Perform statistical analysis
9. Determine optimal solution



Small Boat Attack Problem Revisited*
Custom/Optimal Design

Design

Run	PBS	Fin	C4ISR	F/Fx	Ps
1	L4	L3	L2	L1	0.39
2	L1	L4	L4	L1	0.71
3	L1	L1	L1	L1	0.53
4	L2	L2	L3	L1	0.76
5	L4	L1	L2	L2	0.26
6	L1	L2	L1	L2	0.61
7	L3	L3	L1	L2	0.69
8	L2	L4	L2	L1	0.82
9	L2	L4	L1	L2	0.81
10	L1	L1	L3	L2	0.54
11	L1	L4	L1	L2	0.71
12	L2	L3	L2	L1	0.61
13	L4	L4	L2	L1	0.68
14	L3	L2	L1	L2	0.8
15	L2	L1	L4	L2	0.62
16	L1	L3	L2	L1	0.59
17	L3	L4	L4	L1	0.77
18	L1	L3	L3	L2	0.58
19	L2	L1	L1	L1	0.63
20	L4	L2	L2	L2	0.63
21	L4	L2	L3	L1	0.64
22	L3	L4	L2	L2	0.76
23	L2	L2	L4	L2	0.77
24	L3	L1	L2	L2	0.7

**** Huynh et al. [2007]***

- **Custom design construct**
  - 4 factors*: *PBS, Fin, C4ISR, and F/Fx*
  - 1 two-factor interaction: *PBS×Fin*
  - *D*-optimality
  - Constructed with *JMP Custom Designer*
- **Efficient model-based design**
  - Only 24 runs for determining factors and active interactions

Design Evaluation

Diagnostics for Assessing Design

Alias Matrix

Effect	PBS*Fin 1	PBS*Fin 2	PBS*Fin 3	PBS*Fin 4	PBS*Fin 5	PBS*Fin 6	PBS*Fin 7	PBS*Fin 8	PBS*Fin 9	PBS*C4ISR 1
Intercept										
PBS 1	0	0	0	0	0	0	0	0	0	-0.01
PBS 2	0	0	0	0	0	0	0	0	0	0.074
PBS 3	0	0	0	0	0	0	0	0	0	-0.11
Fin 1	0	0	0	0	0	0	0	0	0	-0.3
Fin 2	0	0	0	0	0	0	0	0	0	0.048
Fin 3	0	0	0	0	0	0	0	0	0	0.028
C4ISR 1	0	0	0	0	0	0	0	0	0	-0.08
C4ISR 2	0	0	0	0	0	0	0	0	0	0.589
C4ISR 3	0	0	0	0	0	0	0	0	0	-0.14
F/Fx	0	0	0	0	0	0	0	0	0	-0.24
PBS*Fin 1	0	0	0	0	0	0	0	0	0	-0.12
PBS*Fin 2	1	0	0	0	0	0	0	0	0	0.146
PBS*Fin 3	0	1	0	0	0	0	0	0	0	-0.01
PBS*Fin 4	0	0	1	0	0	0	0	0	0	-0.1
PBS*Fin 5	0	0	0	1	0	0	0	0	0	0.06
PBS*Fin 6	0	0	0	0	1	0	0	0	0	0.083
PBS*Fin 7	0	0	0	0	0	1	0	0	0	-0.34
PBS*Fin 8	0	0	0	0	0	0	1	0	0	-0.03
PBS*Fin 9	0	0	0	0	0	0	0	1	0	0.059

Parameter	VIF
Intercept	1.727
PBS 1	2.211
PBS 2	1.112
PBS 3	1.638
Fin 1	1.176
Fin 2	1.475
Fin 3	1.513
C4ISR 1	2
C4ISR 2	2.667
C4ISR 3	2.333
F/Fx	1.5
PBS*Fin 1	1.297
PBS*Fin 2	1.099
PBS*Fin 3	1.257
PBS*Fin 4	1.349
PBS*Fin 5	1.089
PBS*Fin 6	1.697
PBS*Fin 7	1.362
PBS*Fin 8	1.357
PBS*Fin 9	2.143

Design Diagnostics

D Optimal Design

D Efficiency	82.56108
G Efficiency	63.24555
A Efficiency	62.5
Average Variance of Prediction	1.333333
Design Creation Time (seconds)	0

- **Alias matrix**
  - – No confounding of main effects and active two-factor interactions
- **Variance inflation factors (VIF)**
  - – Relative to the orthogonal coding
  - – VIF < 5: no collinearity problem
- ***D*-efficiency**
  - – Orthogonal design: 100%
  - – 80%: nearly orthogonal

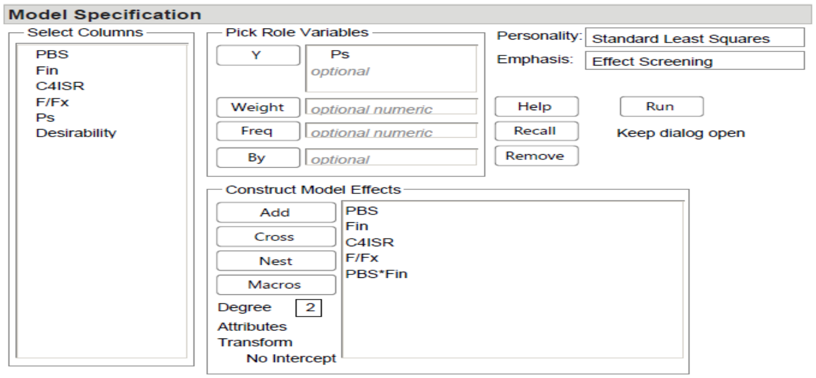
Evaluation of Design

➢ **Very good design**

– Desirable aliasing properties
– Nearly orthogonal
– Small number of runs

Statistical Analysis of Data

JMP *Fit Model Platform*



Fitted MEPTFI Model

Response Ps

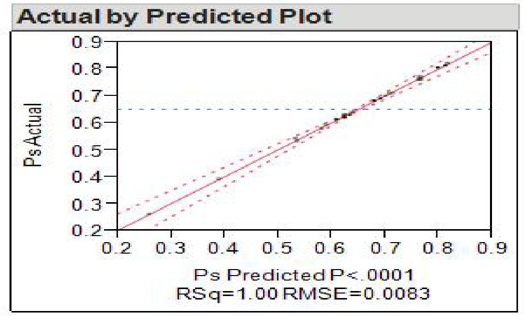
Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	0.6364844	0.002232	285.12	<.0001*
PBS[L1]	-0.025391	0.003544	-7.16	0.0020*
PBS[L2]	0.0667969	0.003139	21.28	<.0001*
PBS[L3]	0.1042969	0.003766	27.69	<.0001*
Fin[L1]	-0.105339	0.003252	-32.39	<.0001*
Fin[L2]	0.0675781	0.003766	17.94	<.0001*
Fin[L3]	-0.067786	0.00362	-18.73	<.0001*
C4ISR[L1]	-0.001667	0.004495	-0.37	0.7296
C4ISR[L2]	-2.6e-17	0.004495	-0.00	1.0000
C4ISR[L3]	-4.73e-17	0.004495	-0.00	1.0000
F/Fx[L1]	0.001875	0.002081	0.90	0.4185
PBS[L1]*Fin[L1]	0.0300781	0.005315	5.66	0.0048*
PBS[L1]*Fin[L2]	-0.06513	0.006337	-10.28	0.0005*
PBS[L1]*Fin[L3]	0.0416927	0.005818	7.17	0.0020*
PBS[L2]*Fin[L1]	0.0270573	0.006001	4.51	0.0107*
PBS[L2]*Fin[L2]	-0.006693	0.005629	-1.19	0.3002
PBS[L2]*Fin[L3]	-0.02737	0.006422	-4.26	0.0130*
PBS[L3]*Fin[L1]	0.0664323	0.007102	9.35	0.0007*
PBS[L3]*Fin[L2]	-0.004818	0.006179	-0.78	0.4791
PBS[L3]*Fin[L3]	0.0205469	0.007461	2.75	0.0512

Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
PBS	3	3	0.13317112	640.8234	<.0001*
Fin	3	3	0.15271885	734.8877	<.0001*
C4ISR	3	3	0.00001667	0.0802	0.9674
F/Fx	1	1	0.00005625	0.8120	0.4185
PBS*Fin	9	9	0.05657607	90.7486	0.0003*

Actual by Predicted Plot



Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	19	0.40161875	0.021138	305.1476
Error	4	0.00027708	0.000069	**Prob > F**
C. Total	23	0.40189583		<.0001*

Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
PBS	3	3	0.13317112	640.8234	<.0001*
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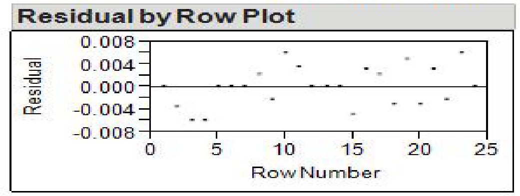
C4ISR	3	3	0.00001667	0.0802	0.9674
F/Fx	1	1	0.00005625	0.8120	0.4185
PBS*Fin	9	9	0.05657607	90.7486	0.0003*

Residual by Row Plot



Analysis of Analysis

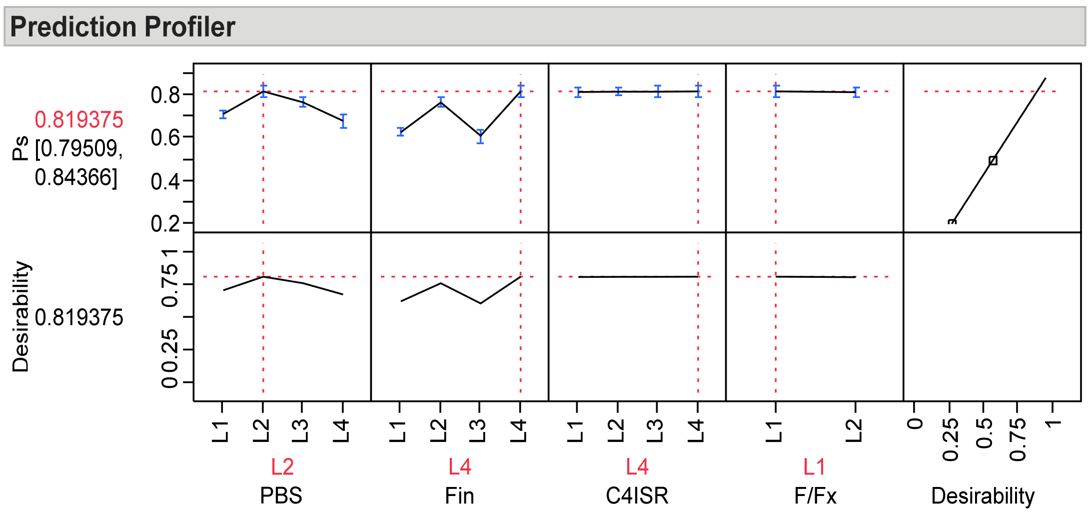
– MEPTFI model has excellent predictive capability

– *PBS*, *Fin*, *PBS×Fin* statistically significant, i.e. $p < 0.05$

– Residual error plot: i.i.d. $N(0, \sigma^2) \Rightarrow$ OLSE applicable

System Allocation Optimization

- **JMP *Prediction Profiler***
  - Determines factor settings that maximize P_S based on fitted MEPTFI model



☞ The "optimal effective" solution differs from the main effects plots of Huynh *et al.* [2007]

☞ ODOE "optimal effective" SBA SoS architecture confirmed using several independent approaches

CAIV Analysis

- **Classical optimal solutions are point solutions**
  – Limited value, precisely wrong
  – Does not take advantage of the full information provided by the simulation experiments

- **Solution: CAIV and/or efficient frontier (EF)**
  – EF and nearby solutions: small set of viable alternatives for rational decision
  – Sound decision based on informative cost-effectiveness comparisons
  – Supports set-based design (SBD) [Singer *et al.*, 2009]

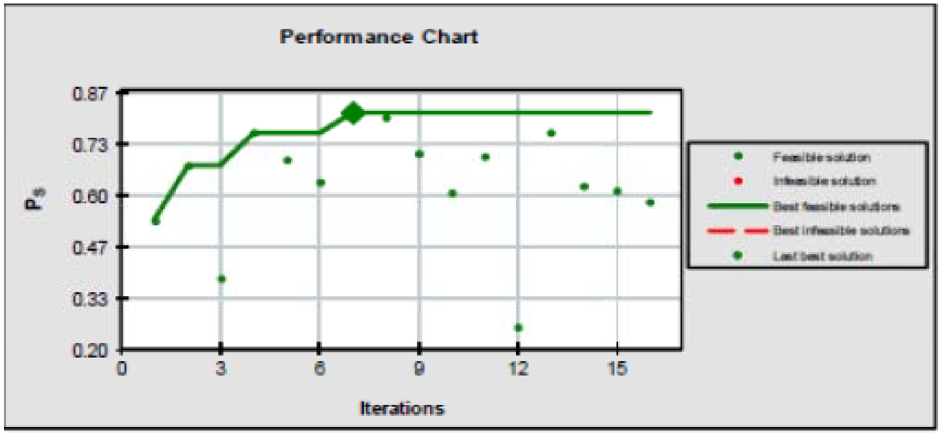
Crystal Ball Report - OptQuest

Run preferences:
  Deterministic optimization (without simulation)
Crystal Ball data:

Objectives	1
Requirements	0
Constraints	4
Linear	4
Decision variables	14
Forecasts	1
" Frozen items "	6

OptQuest Results

Summary:
  After 16 solutions were evaluated in 0 seconds,
  the Mean of PS: was improved from 0.538 to 0.818, a change of 52.16%



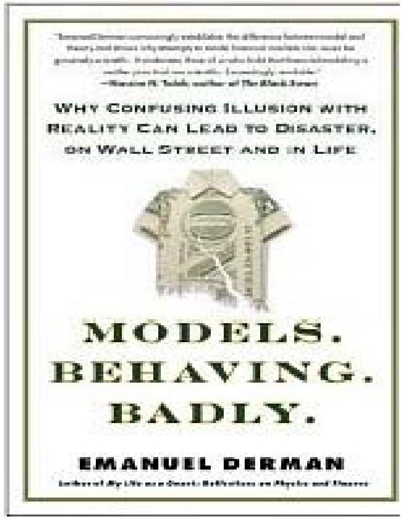
Objectives		Best Solution:	
	Maximize the Mean of PS:	0.818	Cell: C27
Constraints		Left Side:	Right Side:
1	PBS(L1) + PBS(L2) + PBS(L3) + PBS(L4)=1	1.00	1.00
2	Fin(1) + Fin(2) + Fin(3) + Fin(4)=1	1.00	1.00
3	C4ISR(1) + C4ISR(2) + C4ISR(3) + C4ISR(4)=1	1.00	1.00
4	FFx(1) + FFx(2)=1	1.00	1.00

Some Concluding Thoughts (1 of 2)

- **DOE has undergone profound changes in the last 15 years**
  - Significant advances in computing capability and algorithms
  - ODOE: flexible method to design experiments that custom fit circumstances
  - Proven benefits of nearly orthogonal designs with more desirable aliasing
- **MEPTFI model has excellent predictive capability for SoS architecting**
  - Realistic but simple model of interactions between system elements
- **ODOE is well suited for SoS architecting**
  - *D*-optimal design excellent for evaluating main effects and interactions
    - Efficient, reduced number of simulations
    - Simple aliasing
    - Design analysis provides valuable insight
    - Statistical analysis generates metamodel; captures behavior of SoS
  - Implemented in commercial statistical packages
    - JMP Pro, Minitab Pro,...
    - JMP Pro includes true optimization capability
    - Metamodel useful for realistic AoA

Some Concluding Thoughts (2 of 2)

- The application of orthogonal array experiments (OAE) to systems engineering and architecting problems is a significant mistake
  - Systems and SoS ⇒ active interactions ⇒ underlying OAE assumptions outside domain of applicability ⇒ potential for highly misleading results
  - Failure to correct significant mistakes in published works causes harm to both discipline and stakeholders

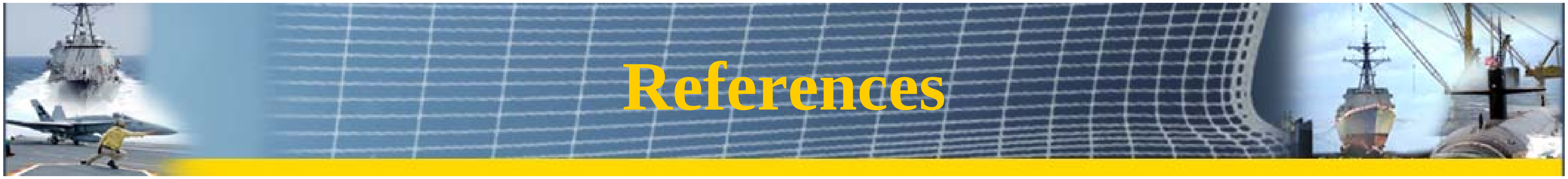


Excerpt of The Modelers' Hippocratic Oath

I will not give the people who use my models false comfort about their accuracy.

I will make the assumptions and oversights explicit to all who use them.

I understand that my work may have enormous effects on society and the economy, many beyond my apprehension.



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