Design of Experiments in Ecological Systems: some methods and issues

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Outline

- Problem statement
- Proposed solution
- Simulation Example
- Some applicable DOEs
- Implementation problems

 and their consequences
- Other modeling issues
- Conclusions

Problem Statement

- Given a network of water masses

 E.g. Finger Lakes, Great Lakes, Gulf Ports
- Optimize some performance measures:
 Wetland Preservation; water use; exports, etc
- Subject to the Key set of economic, social, labor, political, environmental, climatic, cultural, etc. problem variables/constraints
- Maintaining employment, health etc. levels

Modeling Methods

- Theoretical (physics law, or relation)
 - But, can we come up with such equation?
- Empirical (regression)
 - But, can we find enough data to implement?
- Discrete Event Simulation
 - Don't need to relax model assumptions
 - Can include complex interactions
 - But run time can be very long!

Simulation Modeling Problem

- Consider a Complex Simulation Model
- Main Issues:
 - Too many variables to analyze
 - Complex Dynamical System structure
- Proposed solution: Find Key Variables
 - Via Design of Experiments (DOE)
 - Derive a set of simpler Meta Models
 - Use them as proxies for the Full Model

Simulation Example

- Given a network of water masses
 For both, civilian and industrial use
- Optimize some performance measures

 e.g. operational, social, political, ecological
- Subject to a set of (conflicting) political, labor, socio-economic, etc. constraints
 - Maintaining levels of production, employment
 - Tax revenues, social services, economic, etc.

A Network of Interconnected Water Masses



Example: River Port w/Lagoon



Controlled Variables: Economic

- Replenishing Levels (MIN)
- Reservoir Capacity (MAX)
 - Ordering Schedule
 - Transfer Policy
 - Usage Policy
 - Shortage Policy
 - Profitability
- System's Initial Conditions

Controlled Variables: Social

- Allocation to each sector
 - Size of the Reservoirs
 - Transfer Policy
- Generation of electricity
 - Hospitals and schools
 - Transportation uses
 - Recreation uses

Controlled Variables: Ecologic

- Wetland Area
- Wetland Depth
- Transfer Speed
- Water Table Use
 - Pollution Level
- Fish/Foul Population

WetLand v. Level



Uncontrolled Variables

- ECONOMIC
- Political issues
- Labor issues
- Water Theft
- Water Leaks
- Markets
- Financial

- ECOLOGIC
- Evaporation
- Temperature
- Salinity
- Reproduction
- Weather
- Water Table

And Associated Costs

- Of Importing Water from other places
- Transferring from Social to Economic
- Allocation to various constituencies
- Of Water shortages and rationing
- Indirect costs (labor, political, social)
- Ecological costs (degradation, loss)
- Total costs (compound response)

Additional Model Uses

Multi-criteria (ecological, social, economic, etc.) system responses (consolidating elements in the system) can be obtained, by combining (say k) contrasting and competing individual responses into a single, complex one. The (linear) combinations formed quantify the contrasting policies and philosophies of the different constituencies. Comparisons of competing and contrasting policies, via the simulation model results, can help diverse constituencies to rationally discuss their differences, and better reach a consensus.

Simple DOE Example

Complete Factorial Experiment for the Simulation



DOE Model Limitations:

- Analyzes limited variables (here, k=3)
 For, 2^K Factors/Interacts are generated
- The Effect of Interaction, when k > 2

 Can affect results, if present and strong
- Need to find Robust Responses

 Handling specific "noise variables"
- Need to Identify "significant few" variables
 To reduce model Size, maintaining Info level.

And their Consequences ...

- If large number of factors to analyze
 - Strong factor interaction may exist
 - Dependent on the model structure
 - Requires special methods for analysis
- Different objective of models derived:
 To describe/study, forecast or control
- Robust Parameter analysis capability

 To derive a response equation that is
 Resilient to "noise" or uncontrolled factors

Methods for Key Variable Id

- Full Factorial Designs
- Fractional Factorial Designs
- Plackett-Burnam Designs
- Controlled Sequential Bifurcation
- Latin Hypercube Sampling
- Other modeling approaches

– Bayesian, Hierarchical, Taguchi, PCA, etc.

Full Factorials

- Most expensive (in time and effort)
 Prohibitive with current number of factors
- Most comprehensive information

 Provides info on all factor interactions
- Two Examples with a 2^3 Full Factorial
 - First case: mild interaction (AB only)
 - Second: strong and complex interaction
 - Notice how the Model-Estimations vary

2^3 Full Factorial DOE: Variables Used

- A = Replenishing Levels (MIN)
- B = Reservoir Capacity (MAX)
 - C = Transfer Policy
 - Mild interaction assumed
 - A* B only

Full Factorial Experiment 2^3

Run	Α	В	С	Α	B A	C B	C A	BC	Avg.
	1	-1	-1	-1	1	1	1	-1	-1.07
	2	1	-1	-1	-1	-1	1	1	3.72
	3	-1	1	-1	-1	1	-1	1	-0.58
	4	1	1	-1	1	-1	-1	-1	12.04
	5	-1	-1	1	1	-1	-1	1	7.75
	6	1	-1	1	-1	1	-1	-1	15.45
	7	-1	1	1	-1	-1	1	-1	11.09
	8	1	1	1	1	1	1	1	18.31
TotSum									66.71
Effect		8.08	3.75	9.62	1.84	-0.62	-0.65	-2.08	
	Reg	ression Est	imations						
RegCoef	А	В	С	A	В	b0			
Estimat.		4.04	1.88	4.81	0.92	8.34			

Meta Model: $Y_{ijkl} = 8.33 + 4.04A + 1.88B + 4.81C + 0.92AB$

1

10

True Model: $Y = 10 + 4^*A + 2^*B + 5^*C + AB + \varepsilon$

Mild Interaction (AB only)

5

TRUE

4

2

Meta Model Re-creation ability: mild interaction.



Fractional Factorials

- Analyzes only a Fraction of the Full
 - Reduces substantially time/effort
 - Confounding of Main Effects/Interactions
 - If Interactions present, this is a problem
 - Only for Powers of Two (no. of runs)
- Numerical Example: half fractions
 - Of the previous Full Factorial -- and others
 - Assess Model-Estimation agreement

Fractional Factorials

First Fraction: L1

Run		A	4		в	C	C=AB	A	vg.
	1		1		-1		-1		-0.33
	2		-1		1		-1		-0.33
	3		-1		-1		1		-0.33
	4		1		1		1		1.00
TotSum									0.00
Effect		7	7.429		3.130		11.460		
Signif.		No		No		Yes	6		

 $Y_1 = 7.3 + 3.71A + 1.57B + 5.73C^*$

$$Y_2 = 8.33 + 4.36A + 2.18B + 3.89C^*$$

Notice how, by averaging both Half Fraction results, we obtain the Full Factorial results again.

True Model: $Y = 10 + 4^*A + 2^*B + 5^*C + AB + \varepsilon$

Second Fraction: L2 Α Run В C=AB Avg. -1.00 1 -1 -1 -1 2 1 1 -1 0.33 3 -1 1 1 0.33 4 1 0.33 -1 1 TotSum 0.00 Effect 8.728 4.375 7.784 Signif. Yes Yes No

Untangling the Confounded Structure

(L1+L2)/2	8.079	3.753	9.622
(L1-L2)/2	-0.649	-0.623	1.838
Effects	8	4	10

Again 2^3 Full Factorial: Same Variables Used, but now With Strong Interaction

- A = Replenishing Levels (MIN)
- B = Reservoir Capacity (MAX)
 - C = Transfer Policy
 - Strong interaction assumed
 - A*B, A*C, B*C
 - Overall: A*B*C

Full Factorial: Complex, Strong Interaction

	Model I	Parameters					
Variables	Α	В	С	AB	AC	BC	ABC
RegCoef	3	-5	1	-12	8	-10	-15
RegEstim	1.94	-4.38	1.73	-12.14	7.34	-10.52	-15.26
MainEffEst	3.88	-8.76	3.47	-24.28	14.68	-21.05	-30.51
MainEffcts	6	-10	2	-24	16	-20	-30
Var. of Model		12.5173		StdDv	3.53799		
Var. of Effect		2.0862		StdDv	1.44437		
Student T (0.0)25DF)	2.47287					
C.I. Half Widt	h	3.57177					
Factor	Α	В	С	AB	AC	BC	ABC
Signific.	Yes	Yes	No	Yes	Yes	Yes	Yes

True Model and Estimated Meta Model:

Y =	3A -	5B +	C - 2	12AB + 8/	AC - 10BC	- 15ABC
RegEstim	1.94A	-4.38B	1.73C	-12.14AB	+7.34AC -	10.52BC -15.26ABC

Corresponding Half Fractions

		Half	Fraction	Analysis:					
			First	Half(a)					
Run	Α	В	C=AB	Y1	Y2	Y3	Avg.	Var	Model
2	1	-1	-1	-15.03	-16.54	-16.04	-15.87	0.59	-14
3	-1	1	-1	7.18	9.21	5.28	7.22	3.87	6
5	-1	-1	1	-16.75	-19.75	-22.02	-19.51	6.97	-22
8	1	1	1	-31.61	-27.62	-33.04	-30.76	7.89	-30
TotSum				-56.21	-54.7	-65.82	-58.91	19.32	
Effect	-17.17	5.92	-20.81		ModlVar.	4.83	StdDev=	2.2	EffVar
<u>.</u>					7/075 10		<u></u>	2.40	61 ID
Signif.	Yes	Yes	Yes		1(.975,df)	2.75	CI-HW=	3.49	StdDev

Second Half(b)

Run		Α	В	C=-AB	Y1	Y2	Y3	Avg.	Var	Model
	1	-1	-1	-1	-5.64	-0.28	9.43	1.17	58.32	2
	4	1	1	-1	4	1.47	2.49	2.65	1.62	2
	6	1	-1	1	49.73	54.94	56.86	53.84	13.62	54
	7	-1	1	1	5.99	7.88	2.56	5.48	7.26	2
TotSum					54.08	64.01	71.34	63.14	80.82	
Effect		24.92	-23.44	27.75		ModlVar.	20.2	StdDev=	4.49	EffVar
Signif.		Yes	Yes	Yes		T(.975,df)	2.75	CI-HW=	7.14	StdDev
(a+b)/2		3.88	-8.76	3.47	MainEff	"C"				
(a-b)/2		-21.05	14.68	-24.28	Interact	C=AB				
Coefs		6	-10	2						

NOTE: FRACTIONAL FACTORIAL RESULTS, GIVEN THE STRONG INTERACTIONS, ARE POOR.

Plackett-Burnam (PB) DOEs

- A Fractional Factorial (FF) DOE
- Analyses "holes" between adjacent FFs
- Reduces time/effort, considerably
- Confounding of Main Effects/Interactions
- Numerical Example: 11 main effects

 Compare PB to a 2^11 Full Factorial
 Not all Interactions are strong/significant
- Counter Example: strong interactions

Plackett-Burnam w/o Interaction

- A=Replenishing Levels (MIN)
- B=Reservoir Capacity (MAX)
 - C=Ordering Schedule
 - D=Transfer Policy
 - E=Allocation to each sector
 - F=Size of the Reservoirs
 - G=Generation of electricity
 - H=Hospitals and schools
 - I=Wetland size
 - J=Water Table
 - K=Fish/Foul Population

Placket-Burnam Design (no interaction)

Run	А	В	C	C) E	E F	- (G F		J	J I	<	Avg
	1	1	-1	1	-1	-1	-1	1	1	1	-1	1	36.14
	2	1	1	-1	1	-1	-1	-1	1	1	1	-1	24.39
	3	-1	1	1	-1	1	-1	-1	-1	1	1	1	0.5
	4	1	-1	1	1	-1	1	-1	-1	-1	1	1	-5.96
	5	1	1	-1	1	1	-1	1	-1	-1	-1	1	2.62
	6	1	1	1	-1	1	1	-1	1	-1	-1	-1	31.26
	7	-1	1	1	1	-1	1	1	-1	1	-1	-1	21.12
	8	-1	-1	1	1	1	-1	1	1	-1	1	-1	-10.54
	9	-1	-1	-1	1	1	1	-1	1	1	-1	1	15.92
	10	1	-1	-1	-1	1	1	1	-1	1	1	-1	12.02
	11	-1	1	-1	-1	-1	1	1	1	-1	1	1	7.33
	12	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	11.66
Factors	5	Α	В	С	D	E	F	G	н	I	J	К	Во
RegCo	ef	6	2	0	-4	-6	0	-2	4	8	-8	0	12
RegEst.		4.5	2.3	-0.1	-4.3	-3.6	1.4	-0.8	5.2	6.1	-7.6	-2.8	12.2
MainEf	f	12	4	0	-8	-12	0	-4	8	16	-16	0	n/a
EstimEf	f	9.1	4.7	-0.2	-8.6	-7.2	2.8	-1.5	10.4	12.3	-15.2	-5.6	12.2
Signific.		Yes	Yes	No	Yes	Yes	No	No	Yes	Yes	Yes	Yes	Yes

Meta Model Forecasting Ability



Actual by Predicted Plot



Plackett-Burnam with Interaction

- A=Replenishing Levels (MIN)
- B=Reservoir Capacity (MAX)
 - C=Ordering Schedule
 - D=Transfer Policy
 - E=Allocation to each sector
 - F=Size of the Reservoirs
 - G=Generation of electricity
 - H=Hospitals and schools
 - I=Wetland size
 - J=Water Table
 - K=Fish/Foul Population

Model with Moderate Interaction structure:

Factors	Α	В	С	D	Ε	F	G	н	I	J	К	Во
RegCoef	6	2	0	-4	-6	0	-2	4	8	-8	0	12

Interaction: 2*A*B-4*H*I+G*J+D*E

Plackett-Burnam (n=12 rows) Analysis Results:

Factors	Α	В	С	D	E	F	G	н	I	J	К
MainEff	12	4	0	-8	-12	0	-4	8	16	-16	0
FacEstim	-98.6	61.1	41.3	-86.5	98.4	66.4	79.7	51.8	-26.6	37.6	-96.0
RegPar.	6	2	0	-4	-6	0	-2	4	8	-8	0
RegEstim	-49.3	30.5	20.6	-43.2	49.2	33.2	39.8	25.9	-13.3	18.8	-48.0
Signific.	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes

Results are seriously confounded and numerically erroneous.

Meta Model Forecasting Capabilities



Controlled Sequential Bifurcation

- Method to Identify significant Main Effects
- Requires prior knowledge of Effect signs

 To ensure all effects are in same direction
 Requirement is unrealistic in most cases
- Branch and Bound-like approach
 Top-Down approach most often
- Adaptive procedure to assess estimations
 Using the approach but not the method

There are two groups of significant variables after Plackett-Burnam: <u>Positive</u>: B, C, E, F, G, H, J; and Negative: A, D, I, K.

We Perform a Resolution IV FF To one of the two groups

Plackett-Burnam Result Group of "Positive" Vars: B, C, E, F, G, H, J;

- B=Reservoir Capacity (MAX)
 - C=Ordering Schedule
 - E=Allocation to each sector
 - F=Size of the Reservoirs
 - G=Generation of electricity
 - H=Hospitals and schools
 - J=Water Table

Performing a Resolution IV FF to the "Positive" group: B, C, E, F, G, H, J

Factors	В	С	E	F	G	н	J	Во
TRUE	12	4	0	-8	-12	0	-4	12
EffectEstim	12.14	2.53	1.17	-7.20	-11.82	0.39	-3.49	13.59
RegCoef	6	2	0	-4	-6	0	-2	12
RegEst.	6.07	1.26	0.59	-3.60	-5.91	0.19	-1.75	6.80
Signific.	Yes	Yes	No	Yes	Yes	No	Yes	

Notice how, once all the Plackett-Burnam (erroneously estimated) variables of the "same sign" were re-analyzed as a sub-group, estimations became closer to True values, both in sign and in magnitude.

Descriptive ability of the model improves; But its Forecasting capability deteriorates.



Latin Hypercube Sampling

- Multiple regression analysis approach
 Sampling at "best" points in sample space
- Regression selection methods

 To obtain most efficient Meta Model set
- Provides a list of Alternative Meta Models

 Some, not as efficient -but close enough
 Their factors can be "controlled" by the user
- Very effective modeling approach.

Latin Hypercube Example

Assume we have a three dimensional (p = 3) problem in variables B, I, J (reservoir capacity; wetland size and water table use) and that these are respectively distributed Normal, Uniform and Exponential,. Assume that we want to draw a random sample of size n = 10. Divide each variable, according to its probability distribution, into ten equi-probable segments (Prob. = 0.1 = 1/10), identifying each segment with integers 1 through 10. Then, draw a random variate (r.v.) from each of the ten segments, for each of the three variables B, I, J. Finally, obtain the 10! permutations of integers 1 through 10. Randomly assign one of such permutations (e.g. segments 2,1,5,4,6,9,8,10,7 for B), to each of the variables, select the corresponding segment r.v., and form the vector sample, as below:

Example of Latin Hypercube Sampling Segments

Sample	1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th
В	2	3	1	5	4	6	9	8	10	7
Ι	4	2	7	1	5	9	10	8	6	3
J	8	6	2	7	1	5	4	3	9	10

Latin Hypercube Example

- Air Force Iraq Simulation Model
 - Fifty plus model variables
 - Two different responses of interest
 - Identify the Key or Relevant Few
 - Preserve as much Info as possible
- Analysis Results
 - Three Key Variables were identified
 - Ninety Percent of the Info ($R^2 = 0.9$)

Regression Selection Analyses Results

SUMMARY OUTPUT

Regression Statistics				
R Square	0.974347			
Observations	450			

SUMMARY OUTPUT:

R Square	0.854967
Observations	450

	Coeff	P-value
Intercept	0.034007	0.218928
X Variable 1	-3.00E-05	3.70E-193
X Variable 2	3.94E-05	0

	Coef	P-value
Intercept	6.158105	1.26E-07
X Variable 1	0.000251	6.90E-75
X Variable 2	-0.00026	4.90E-143
X Variable 3	0.047911	1.96E-05
X Variable 4	-1.46362	1.09E-62

SUMMARY OF IMPROVED META MODELS DERIVED:

RESPONSE	KEY VARIABLES	INDEX OF FIT	F-STATISTIC
ECONOMIC	AH, AK, AM, AR	97,6%	4723.7
ECONOMIC	AH, AK	97.4%	8488.9
VIOLENCE	AH, AK, AM, AR	85.5%	655.8
VIOLENCE	AH, AK, AR, AX	85.1%	637.5
VIOLENCE	AH, AK	72.4%	587.5
VIOLENCE	AH,AK,AM,AP,AR,AS,AT, AU,AV,AW	94.8%	800.4

CORRELATION MATRIX FOR THE FOUR COMMON KEY VARIABLES AND THE TWO RESPONSES:

	KEYVAR 1	KEYVAR 2	Column 3	Column 4	Violent	Econ
KV 1	1					
KV 2	-0.07464	1				
Col 3	0.00345	0.088232	1			
Col 4	0.032984	0.0929	0.055228	1		
Violence	0.44621	-0.7560	-0.0018	-0.4056	1	
Econ	-0.4637	0.90353	0.028	0.08433	-0.8671	1

Principal Components

- Can also be used with Latin Hypercube
 - When variables are strongly correlated
 - Alternative dimension reduction technique
- Main problem: how to interpret it:
 - To identify Key variables through loadings?
 - To use the PCA Main Factors, instead?
 - Alternative approaches?
- Needs evaluation and comparison w/DOE

Example of Varimax Factor Rotation ·	Variable	Factor1	Factor2
P_{rest}	x1	0.930	0.030
Project variables X1 and X2 on F1	x2	0.883	-0.249
Then, Project Variable X3 on Factor 2.	x3	-0.097	0.989



Other Approaches

- Bayesian
 - Assume a prior on Meta Model terms
- Hierarchical
 - Sub-model output yields upper level input
- Taguchi
 - Derive results resilient to "noise" parameters
 - Parameters representing "uncontrolled" vars
 - Provides many conceptual DOE ideas.

Taguchi Approach

- Analyzes both Location and Variation
 Of the performance measure of interest
- Best combination of both these together
 To obtain most efficient Meta Model
- Optimize Location, resilient to Variation
- Minimize Variation, resilient to Location
- Determine regions of joint optimality
- Determine Variation is Not an issue
- Can be equivalently implementing w/DOE



Example of Taguchi

- Response: Wet Land Size
- X1=Reservoir Capacity (MAX)
 - X2=Generation of electricity
 - X3=Hospital Capacity
 - X4=Social Services
 - X5=Fish/Foul Population

Comparison of *Combined* DOE and Taguchi's Approach

X1	Х3	X2	X4	X5	1	2	3	4	Var	LnVar	Average	TagMinim
1	1	1	-1	-1	194	197	193	275	1616.25	7.39	214.75	-46.75
1	1	-1	1	1	136	136	132	136	4.00	1.39	135.00	-42.61
1	-1	1	-1	1	185	261	264	264	1523.00	7.33	243.50	-47.81
1	-1	-1	1	-1	47	125	127	42	2218.92	7.70	85.25	-39.51
-1	1	1	1	-1	295	216	204	293	2376.67	7.77	252.00	-48.15
-1	1	-1	-1	1	234	159	231	157	1852.25	7.52	195.25	-45.97
-1	-1	1	1	1	328	326	247	322	1540.25	7.34	305.75	-49.76
-1	-1	-1	-1	-1	186	187	105	104	2241.67	7.71	145.50	-43.59



Regression Analysis for the Main Effect influence

	Coef	Std Err	t Stat	P-value	Lower 95	Upper 95
Intrcpt	197.13	7.88	25.01	0.00	181.00	213.25
X Var 1	-27.50	7.88	-3.49	0.00	-43.62	-11.38
X Var 2	56.88	7.88	7.21	0.00	40.75	73.00

Regression Analysis for the Variance Influence

	Coef	Std Err	t Stat	P-value	Lower 95	Upper 95
Intrcpt	6.77	0.78	8.70	0.00	4.77	8.77
X Var 1	-0.82	0.78	-1.05	0.34	-2.82	1.18
X Var 2	0.69	0.78	0.88	0.42	-1.31	2.69



Optimal Solution:

Overlaying both plots (for location and variation) we seek to Minimize both Yield (Errors) and Variation.

Jointly applying the two above (cols. 3 & 8).

Estimated Yield:

Y = 197.12 - 27.5X1 + 56.9X2 Y (1, -1) = 112.72

Estimated Variation:

 The Optimum is around (1, -1), yielding
 Y = 6.77 - 0.82X1 + 0.69X2

 Estimated Minimum Output = 113; Min Variation = 5.3
 Y (1, -1) = 5.26

Alternative Combined DOE Approach

Some Applications

- Model Size Reduction for:
- Evaluation of Decisions and Strategies
- Evaluation of Robust Strategies
- Trade-offs and Sensitivity analyses
- What-if, time to catastrophic fails, etc.
- Design and Optimization of Systems
- Study of key Factors on a System
- Arbitration and Conflict Resolution

Composite Objective Functions

Ecologic: Xi is number of occurrences of ith item:

$$f(x_1, \dots, x_p) = \sum_i v_i x_i; with : \sum v_i = 1$$

Economic: Yi = aiXi is cost of No. ith item occurrences:

$$g(x_1, \dots, x_p) = \sum_{i} \lambda_i y_i; with : \sum_{i} \lambda_i = 1$$
$$l(w_1, \dots, w_n) = \sum_{i} \delta_i w_i; with : \sum_{i} w_i = 1$$

Arbitration and Trade-Off: α is the preference or weight:

$$H(g,l) = \alpha g + (1 - \alpha)l; with : 0 < \alpha < 1$$

Example of approach use:

- Reduce Model to Key Variables to:
- Minimize Total Water Operations Cost
- Subject to:
 - Maintaining specified labor levels
 - Reducing pollution to specified levels
 - Maintaining specified social levels
 - Maintaining specified consumption levels
 - Increasing overall health indices

Trade-Off Examples

Scenario	Ecologic	Health	Industry	Education	Recreation	Other
Best Ecologic Best Health	X1 X2	Y1 Y2	Z1 Z2	W1 W2	L1 L2	M1 M2
Best Industry	Х3	A	nalyze Ma	axi-min and		
Best Education	X4		Mini-ma	x results		
Best Recreation	Х5					

Best Other X6

Conclusions

- A very complex problem
 - Size and interactions are serious issues
- Existing methods, not fully compliant
 - But a promise if worked around
- Meta Models extremely useful
 - For strategic and tactical decisions
 - In crisis, and to assess/avoid them
 - In theoretical studies.