

Conference Organization and Goals

**Bruce Ankenman & Barry Nelson (Northwestern Univ.),
Derek Bingham (Simon Fraser Univ.),
Angela Dean & Thomas Santner (Ohio State Univ.)**
**A Workshop of the INI Programme on the
Design and Analysis of Experiments**

5 September 2011

Outline

- 1 Physical Experiments
- 2 Computer Experiments
- 3 Workshop

- All of the participants of this workshop use experimentation

- All of the participants of this workshop use experimentation
- Many communicate minimally - different experimental modalities, and application areas

- All of the participants of this workshop use experimentation
- Many communicate minimally - different experimental modalities, and application areas
- Historically, experimental modalities developed:

1 Physical Experiments

- All of the participants of this workshop use experimentation
- Many communicate minimally - different experimental modalities, and application areas
- Historically, experimental modalities developed:
 - 1 **Physical Experiments**
 - 2 **Stochastic Computer Experiment**

- All of the participants of this workshop use experimentation
- Many communicate minimally - different experimental modalities, and application areas
- Historically, experimental modalities developed:
 - 1 **Physical Experiments**
 - 2 **Stochastic Computer Experiment**
 - 3 **Deterministic Computer Experiments**

Outline

- 1 Physical Experiments
- 2 Computer Experiments
- 3 Workshop

- **Physical Experiments** are the **gold-standard** for determining the relationship between a endpoint of scientific interest and factors that may affect it.

- **Physical Experiments** are the **gold-standard** for determining the relationship between a endpoint of scientific interest and factors that may affect it.
- **Some Features of Physical Experiments**

- **Physical Experiments** are the **gold-standard** for determining the relationship between a endpoint of scientific interest and factors that may affect it.
- **Some Features of Physical Experiments**
 - **Expensive** to run hence **few factors**, each with few levels and restricted run sizes.

- **Physical Experiments** are the **gold-standard** for determining the relationship between a endpoint of scientific interest and factors that may affect it.
- **Some Features of Physical Experiments**
 - **Expensive** to run hence **few factors**, each with few levels and restricted run sizes.
 - **Blocking factors** allow the experimenter to broaden the inference about the **primary treatment factors** to **multiple environments**.

- **Physical Experiments** are the **gold-standard** for determining the relationship between an endpoint of scientific interest and factors that may affect it.
- **Some Features of Physical Experiments**
 - **Expensive** to run hence **few factors**, each with few levels and restricted run sizes.
 - **Blocking factors** allow the experimenter to broaden the inference about the **primary treatment factors** to **multiple environments**.
 - **Randomization** is used to prevent factors that are not recognized by the experimenter from systematically affecting treatment comparisons.

Physical Experiments

- The **experimental design** (including the choice of sample size) is selected
 - to allow independent estimation of model parameters,

Physical Experiments

- The **experimental design** (including the choice of sample size) is selected
 - to allow independent estimation of model parameters,
 - for Screening,

Physical Experiments

- The **experimental design** (including the choice of sample size) is selected
 - to allow independent estimation of model parameters,
 - for Screening,
 - to allow efficient comparison of (scientifically important) treatment contrasts,

Physical Experiments

- The **experimental design** (including the choice of sample size) is selected
 - to allow independent estimation of model parameters,
 - for Screening,
 - to allow efficient comparison of (scientifically important) treatment contrasts,
 - to facilitate prediction

Physical Experiments

- The **experimental design** (including the choice of sample size) is selected
 - to allow independent estimation of model parameters,
 - for Screening,
 - to allow efficient comparison of (scientifically important) treatment contrasts,
 - to facilitate predictionamong other goals

Outline

- 1 Physical Experiments
- 2 Computer Experiments**
- 3 Workshop

Computer Experiments

- **Computer experiments** use of computer simulator of an input/output relationship in place of a physical system

Computer Experiments

- **Computer experiments** use of computer simulator of an input/output relationship in place of a physical system
- **Computer simulators**
 - **Stochastic**
 - **Deterministic**

Stochastic Computer Simulations (SCS)

- SCSs typically used to understand **Discrete Event Dynamic Systems**

Stochastic Computer Simulations (SCS)

- SCSs typically used to understand **Discrete Event Dynamic Systems**
- **Majority use Macro-Modeling**
 - Queueing models: traffic-auto, airport scheduling of Cargo and Passenger, computer networks, . . .
 - Inventory Simulations (output costs and fill rates)
 - Production planning models

Stochastic Computer Simulations (SCS)

- SCSs typically used to understand **Discrete Event Dynamic Systems**
- **Majority use Macro-Modeling**
 - Queueing models: traffic-auto, airport scheduling of Cargo and Passenger, computer networks, . . .
 - Inventory Simulations (output costs and fill rates)
 - Production planning models
- **Applications in** Business Management; Manufacturing; Management; Military Applications; Network analysis; Risk Analysis

Stochastic Computer Simulations

- **Output** is **random**: Waiting times (for manufacturing, passenger or cargo delivery, product development); Cost; Measures of product/process quality

Stochastic Computer Simulations

- **Output** is **random**: Waiting times (for manufacturing, passenger or cargo delivery, product development); Cost; Measures of product/process quality
- Output is real-valued, multivariate, or functional time series

Stochastic Computer Simulations

- **Output** is **random**: Waiting times (for manufacturing, passenger or cargo delivery, product development); Cost; Measures of product/process quality
- Output is real-valued, multivariate, or functional time series
- **Input Variables**
 - Environmental (modeled stochastically)
 - Model (Input uncertainty)
 - Controllable

Stochastic Computer Simulations

- **Typical Scientific Goals**
 - Model verification
 - Screening
 - Sensitivity Analysis, to quantify the effects of individual inputs and joint effects of sets of inputs
 - Determine robustness of model output to random environmental or uncertain model inputs (components)
 - Choice of control variables to optimize system performance

Stochastic Computer Simulations

- **Interface with Classical Statistical Methodology**
(Weighted) Regression analysis; Xvalidation and Bootstrap methodology; Design: orthogonality, resolution, aliasing patterns

Deterministic Computer Simulators

- **Numerical implementations** of a (or more) physics- or biology-based **mathematical model** relating input-output relationship.

Deterministic Computer Simulators

- **Numerical implementations** of a (or more) physics- or biology-based **mathematical model** relating input-output relationship.
- **Use Micro-modeling**: Often Coupled PDEs

Thus consider the linear biphasic equations in the form appropriate to these field variables:

$$\begin{aligned} (v'_i - \kappa p_{,i})_{,i} &= 0 \\ \sigma_{ij}^{tot} &= (\sigma_{ij}^s + \sigma_{ij}^f)_{,j} = (C_{ijkl} u'_{k,j} - \delta_{ij} p_{,i})_{,j} = 0 \end{aligned} \quad (1)$$

where κ is the permeability, $(\cdot)_{,i}$ denotes the partial derivative, σ_{ij}^α , $\alpha = s$ and $\alpha = f$ are the respective solid and fluid phase stress tensors, p is the fluid phase pressure, $\varepsilon_{ij} = u'_{i,j}$ is the solid phase strain tensor (the superscript s is omitted), defined in terms of solid phase displacements, u'_i , C_{ijkl} is the material property tensor of the solid phase, δ_{ij} is the Kronecker delta, $v'_i = \frac{du'_i}{dt}$ is the solid phase velocity, and $\sigma^{tot} = \sigma^s + \sigma^f$ is the total stress. The solid phase and fluid phase stress tensors are defined as:

$$\begin{aligned} \sigma_{ij}^s &= C_{ijkl} u'_{k,j} - \phi^s p \delta_{ij} \\ \sigma_{ij}^f &= -\phi^f p \delta_{ij} \end{aligned} \quad (2)$$

where ϕ^s, ϕ^f are the solid and fluid volume fractions, respectively, for the saturated ($\phi^s + \phi^f = 1$) mixture.

With these phase stress definitions, the total stress, σ_{ij}^{tot} is

$$\begin{aligned} \sigma_{ij}^{tot} &= \sigma_{ij}^s + \sigma_{ij}^f = C_{ijkl} u'_{k,j} - \phi^s p \delta_{ij} - \phi^f p \delta_{ij} \\ &= C_{ijkl} u'_{k,j} - (\phi^s + \phi^f) p \delta_{ij} \\ &= C_{ijkl} u'_{k,j} - \delta_{ij} p = \sigma_{ij}^s - \delta_{ij} p \end{aligned} \quad (3)$$

Deterministic Computer Simulators

- **Applications in** climatology, cosmology (physical experiments are limited), engineering (decrease lead times), biomechanics and many life sciences (ethical constraints), economics

Deterministic Computer Simulators

- **Applications in** climatology, cosmology (physical experiments are limited), engineering (decrease lead times), biomechanics and many life sciences (ethical constraints), economics
- **Output is deterministic** (up to numerical noise): stresses and/or strains in materials; Pressures; Time for some event to occur

Deterministic Computer Simulations

- **Inputs**
 - Environmental (modeled stochastically)
 - Model (Input uncertainty)
 - Controllable

Deterministic Computer Simulations

- **Inputs**
 - Environmental (modeled stochastically)
 - Model (Input uncertainty)
 - Controllable
- **Typical Scientific Goals**
 - Model verification (does the FE, CFD, or other numerical method solve the mathematical model)
 - Screening
 - Sensitivity Analysis, to quantify the effects of individual inputs and joint effects of sets of inputs

Deterministic Computer Simulations

- If data from an analogous physical experiment is available, assess bias in computer simulator; calibrate the computer simulator; predict the output from future physical experiments
- Choice of control variables to optimize system performance (mean performance for the proposed environment)

Outline

- 1 Physical Experiments
- 2 Computer Experiments
- 3 Workshop**

Goals and Workshop

- Learn about details of each communities' research and applications

Goals and Workshop

- Learn about details of each communities' research and applications
- Share perspectives for solving using and fusing our experimental methodologies

Goals and Workshop

- **Workshop**

- Day 1**
- 1 Substantive applications from members of the computer simulation communities
 - 2 Validation and calibration methodology
 - 3 In Session on Computer Simulators and Physical Experiments I, Grant Reinman will speak on “Design for Variation”
 - 4 Poster Storm/Preview
 - 5 RVP Lecture on Orthogonal Arrays (wine reception)

Goals and Workshop

- Day 2**
- 1 Design
 - 2 Panel Discussion #1– Interfacing Physical and Computer Experiments
 - 3 Screening

Goals and Workshop

Day 2

- 1 Design
- 2 Panel Discussion #1– Interfacing Physical and Computer Experiments
- 3 Screening

Day 3

- 1 Large-scale SCS
- 2 Use of Kriging Methodology in SCS
- 3 Free time to Tour Cambridge

Goals and Workshop

- Day 4**
- 1 Input uncertainty, Robustness and UQ
 - 2 Kriging and related methodology
 - 3 Panel Discussion #2–Input uncertainty and experimental robustness

Goals and Workshop

- Day 4**
- 1 Input uncertainty, Robustness and UQ
 - 2 Kriging and related methodology
 - 3 Panel Discussion #2—Input uncertainty and experimental robustness
- Day 5**
- 1 Prediction methodology: multiple models, UQ,
 - 2 Panel Discussion #3: What have heard? What are the common challenges to our research communities? (Qua es nos iens?)

Caius Dining Hall

