Scientific Method vs. Engineering Method

**Engineering Method**
- **Model**
  - Construction
  - Verification
  - System

**Scientific Method**
- **Model**
  - Discovery
  - Falsification
  - System

**Direct Engineering**

**Reverse Engineering**
Scientific Method vs. Engineering Method

**Engineering Method**
- Model
- System
- Direct Engineering

**Scientific Method**
- Model
- System
- Reverse Engineering

“Truth” vs. “Never Correct”
Scientific Method vs. Engineering Method

**Engineering Method**

- **Model**
  - Construction
  - Verification

- **System**
  - Direct Engineering

**Scientific Method**

- **Model**
  - Surprising models
    - Engineering (Computing) -inspired models
  - Surprising systems
    - Nature (Biology) -inspired systems

- **System**
  - Reverse Engineering

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Scientific Method vs. Engineering Method

The models that we discover should be suitable for construction.

The systems that we build should be suitable for discovery.

Model

System

Combined Method

Construction

Verification

Discovery

Falsification
Scientific Method vs. Engineering Method

**Engineering Method**

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**Scientific Method**

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**This Talk**

- Engineering (Computing) -inspired models
- Surprising models (don’t “fix” it, build it!)
- Nature (Biology) -inspired systems
- Surprising systems (don’t “fix” it, understand it!)
The Program and the State Space

The “program”:

The “state space”:

Finite

Potentially infinite
These diagrams commute via appropriate maps.

L. Cardelli: “On Process Rate Semantics” (TCS)
L. Cardelli: “A Process Algebra Master Equation” (QEST'07)
- Run “the program” through a walk in states space.

- **Basic stochastic algorithm: Gillespie**
  - Exact (i.e. based on physics) stochastic simulation of chemical kinetics.
  - Can compute concentrations and reaction times for biochemical networks.

- **Stochastic Process Calculi**
  - Now may [BioSPi, SPiM, BioPEPA, BetaBinders, ...]

- **Hybrid approaches**
  - Continuous + discrete/stochastic switching
Control Flow Analysis

- Who called who?
  - Overapproximation of behavior used to answer questions about what “cannot happen”.

What event may (or may not) have been involved in reaching this state?
Causality Analysis

- What event caused what other event or state to happen?
- Need a different level of representation (the “event space”)
  - Petri Nets
  - Event Structures

What event “caused” this state?
Abstract Interpretation

- Precisely relating abstract views to more concrete views of the system

May now be finite!
Modelchecking

- Asking questions (in Temporal Logic) about structure of a (finite) state space.

- Various flavors of modelchecking:
  - Temporal
    - About paths through state space
  - Quantitative
    - About quantitative measures of states
  - Probabilistic/Stochastic
    - About probabilities of reaching states.

Is this state a necessary checkpoint to reach this state?
- Biology (unlike much of chemistry) is combinatorial
  - Biochemical systems have many regular repeated components
  - Components interact and combine in complex combinatorial ways
  - Components have local state
  - A biochemical system is vastly more compact than its potential state space

- One may expand the state space during analysis, but must not do it during description

- There is a good way:
  - Describe biochemical systems compositionally
  - Each component with its own state and interactions
  - ... as Nature intended...
Conclusions

- **Connections between modeling approaches**
  - Connecting the *discrete/concurrent/stochastic/molecular* approach
  - to the *continuous/sequential/deterministic/population* approach

- **Connecting syntax with semantics**
  - **Syntax** = model presentation (equations/programs/diagrams/blobs etc.)
  - **Semantics** = state space (generated by the syntax)

- **Ultimately, connections between analysis techniques**
  - We need (and sometimes have) good semantic techniques to analyze state spaces (e.g. calculus, but also increasingly modelchecking)
  - But we need equally good **syntactic techniques** to structure complex models (e.g. compositionality) and analyze them