Challenges in Simulation

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Unification of discrete and continuous simulation

Ensembles as the top level unit of simulation

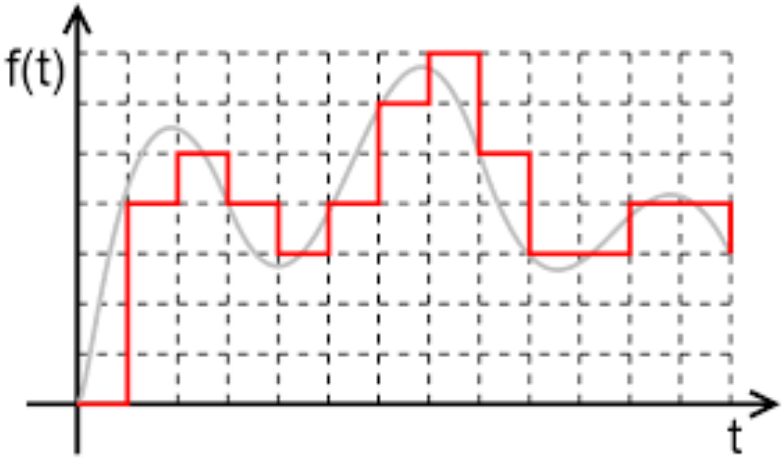
We have no theory for how to combine or couple discrete and continuous simulations!

Complex simulations often have both *continuous* and *discrete* components

- **controlled systems (aircraft, auto engine, power grid)**
- **materials continuous at coarse scale, discrete at fine scale**

Examples are ubiquitous

But surprisingly, we have no comprehensive theory for how to combine, or even couple discrete and continuous simulations



Two different simulation worlds

Continuous simulation

- ***Differential equation*** **defines system behavior; simulation is trying to "solve" the equation**
- **State change *continuous***
- **Models are deterministic; generally no statistical issues**
- **Numerical convergence, accuracy and stability are central issues**
- **Parallel simulations generally time-stepped,**
- **Expertise primarily confined to applied mathematicians**

Discrete simulation

- ***No equation*****; often no general formalism describing system behavior outside of the code**
- **State changes *discontinuous***
- **Many models probabilistic; statistical issues critical in ensemble studies**
- **No numerical issues**
- **Parallel simulations often event-driven, and synchronized by conservative or optimistic algorithms**
- **Expertise mostly held by non-mathematicians**

How to proceed wuth unification of continuous and discrete simulation

- **Time-stepped continuous simulators for ODE and PDE integration must be (re)designed for coupling to discrete event simulations.**
- **Develop the numerical analysis theory of variable rate integrators**
- **Create variable-rate integrators that are directly in discrete event form, rather than time-stepped.**
- **I suspect the unification will involve making continuous simulations event-driven**

Simulation Ensembles

- **Useful simulations usually have *n* inputs, *p* parameters and *r* random variables**
- **Forms an (*n+p+r*)-dimensional space of model behaviors**
- **The goal of a simulation study is to answer questions about that *space* or *ensemble* of behaviors.**

Ensemble Studies

- parameter optimization
- parameter sensitivity
- exhibit rare combinations of events
- estimate means, variances, other moments and distribution parameters, correlation coefficients, etc.
- estimate frequencies of rare events
- uncertainty quantification
- validation against mathematical models, other simulations, or experiment

Ensemble Studies

- **The goal should be to conduct an entire ensemble study *in a single job on a parallel machine.***
- **Must incorporate a *job control API* into the OS**
  - **Allocate groups of nodes**
  - **Launch whole simulation (sub)jobs in parallel on those groups of nodes (with time limits)**
  - **Be notified when each job completes, normally or abnormally**
  - **Reclaim nodes, and launch more ensemble runs as needed**
- **Current cluster OS's often do not allow remote process creation, let alone remote job initiation and node allocation.**