Artificial Intelligence and Simulation

System Dynamics Conference
Lyle Wallis & Mark Paich
Headlines make it clear that AI is a hot topic...

What does that mean for simulation?

"AI is one of the most important things humanity is working on. It is more profound than, I dunno, electricity or fire."
- Sundar Pichai
Google CEO

"The trajectory of AI and its influence on society is only beginning."
- Satya Nadella
Microsoft CEO

"Artificial Intelligence Is Likely to Make a Career in Finance, Medicine or Law a Lot Less Lucrative"
- Entrepreneur
August 2017

"Just as electricity transformed almost everything 100 years ago, today I actually have a hard time thinking of an industry that I don’t think AI will transform in the next several years."
- Andrew Ng
Google Brain, Baidu, Stanford University

PwC | Artificial Intelligence and Simulation
AI is a collection of techniques and technologies across a number of domains:

**Natural Language**
- Natural Language processing and text mining
- Natural Language generation
- Chatbots and discourse understanding
- Sentiment & emotion analysis
- Speech-to-text and text-to-speech

**Machine Learning**
- Regression & classification
- Bayesian learning
- Probabilistic programming
- Anomaly detection
- Optimization techniques
- Support Vector Machines
- Various supervised, semi-supervised, and unsupervised techniques

**Deep Learning**
- Convolutional Neural Nets
- Recursive Neural Nets
- Capsule Networks
- Generative Adversarial Networks
- Deep reinforcement learning
- Hybrid learning models

**Simulation@Scale**
- Cloud simulation
- Big data architecture
- Cloud ML – AWS, GCP, Azure
- Machine Learning deployment
- DRL Toolchains

**Automated ML**
- Automated data preparation
- Automated feature engineering
- Automated algorithm selection
- Automated explanation generation
- Meta-model inference

**Simulation & RL**
- System dynamics modeling
- Agent-based simulation
- Digital Twins
- Reinforcement learning
- Augmented and synthetic data generation
- Calibration of models

**Embodied AI**
- IoT and Industrial IoT – Edge computing and Smart sensors
- Drone – Autonomy & Image analytics
- Robots – Navigation & Learning
- Brain-Machine Interfaces

**Responsible AI**
- Explainable AI
- Beneficial AI
- ‘Black box’ Interpretability
- Maturity models
- Ethics and Law
- AI Governance
- AI Controls framework
Simulation Development and ML/NLP Model Development
...are fundamentally different

Causal

Human defines set of rules (simulation) which transform the input data into the output

Correlational

Machine infers the model based on large amounts of input and output examples
BodyLogical

Meta-Modeling

Combining Simulation and ML
An individual level, ODE-based, simulation model of the human body used to predict the progression of chronic diseases such as metabolic syndrome using BodyLogical requires calibration for thousands of individuals in a selected population.

- BodyLogical is calibrated to clinical biomarkers (e.g. blood pressure, glucose level, etc) at an individual level.
- Full calibration for an individual uses a differential evolution algorithm that is very time consuming.
  - Multiple days for a 15000 person population
Combining **Simulation** and **Machine Learning** approaches to create a **Meta-Model** accelerates the calibration process.
Using Machine Learning to relate individual bio-markers to previously estimated model parameters, the meta-model accelerates the calibration process.

**Test Data** – Test data is similar to train data but we will not be using it for model training but for evaluating the predictions.

**Train Data** – Dataset contains ~60000 entries. It has biomarkers time course data for 4 times-points between 40-44 age and have corresponding parameters for them.

Use predicted parameters to generate the biomarkers for given timepoints and check the quality of fit for calibration.

Checking the quality of fit.
The meta-model provided an excellent fit between patient biomarkers and previously estimated model parameters. Performance

The meta-model was extremely fast. Parameters for 15,000 individuals could be estimated in 3 seconds.

There were some cases where the meta-model didn’t perform as well. Generally, these were cases where the patient had a major health intervention.

Approach is very promising and is continuing to be pursued.
Example Results

Data without intervention
(Best fit example)
Getting an answer to “So What?”

Combining Simulation with Deep Reinforcement Learning
Deep Reinforcement Learning (DRL) gives us a promising way to do simulation model policy analysis and answer “So What?”

Simulation is great for describing systems, creating shared mental models, and predicting system behavior. However, we often are challenged with “so what?”

Answering “So What?” requires a prescriptive response that in the SD world we call “policy.”

DRL combined with simulation gives us a new way to generate good policies and integrate them into the fabric of the systems themselves.
DRL solves problems that require a complex sequence of actions to optimally reach a desired goal state

- Actions are generated periodically (e.g., every minute, day, year) or a-periodically based on the system reaching a specific state (condition).
- The outcome (i.e., the next observed state of the system) of each action taken is uncertain.
- For every system state the policy Deep NN generates the best action to ultimately reach a goal state, even if that goal state is many decisions (actions) in the future.
- DRL is effective even for systems with immense state spaces.
- This is a Markov Decision Process implemented with simulation, neural nets, and reinforcement learning.
Once a system simulation has been created the **Deep NN “Brain”** is trained using **reinforcement learning (RL)**

- RL works similarly to how humans learn – through exploration and exploitation (aka: **trial and error**)
- The process is guided by a system of **rewards and penalties** towards the desired goal state
- As a rule of thumb it can take ~1 **million simulations** to train the Deep NN. This requires a high performance tool chain to train the NN in reasonable time.
Trained Deep NNs ("brains") embed the entire state-action space of the system and can be deployed independently of the simulation.
Advanced Simulation + DRL tool chains create the capability to deploy and embed policies into operational systems

Strong prescriptive insights combined with deployment options expands the range of application for system simulation and systemic thought

- **Embodied Systems**
  - Robotics
  - Drones
  - Industrial Control

- **Operational Systems**
  - Supply Chain
  - Scheduling
  - Logistics
  - Inventory

- **Strategy**
  - Dynamic and Resilient Strategy
  - Pricing
  - Production
  - Promotion
  - Competitive response
DRL can be advantageous over other techniques for policy analysis in situations where the system is highly non-linear and/or uncertain

**Advantages**

- Inherently multi-period
- Generates adaptive policies
- Effectively handles uncertainty
- Effectively handles non-linear systems
- Scales to very complex systems with very large state spaces
- Computationally cheap once the policy is created
- Policies can be evaluated by observing the state-action response in simulation

**Disadvantages**

- Computationally expensive to create the policy
- Complex tool chains
- Multi-disciplinary set of skills required to execute and deliver
- Policies must be evaluated by observing the state-action response in simulation
Simulation is an integral part of the AI landscape. As AI technologies advance, the opportunities for simulation will increase.
Thank you.