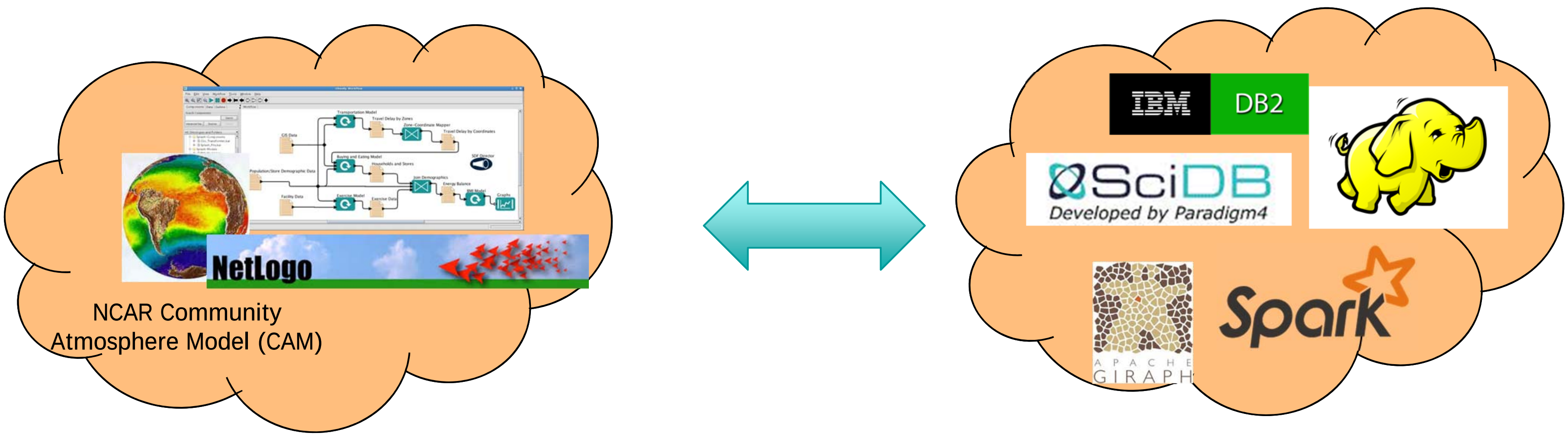
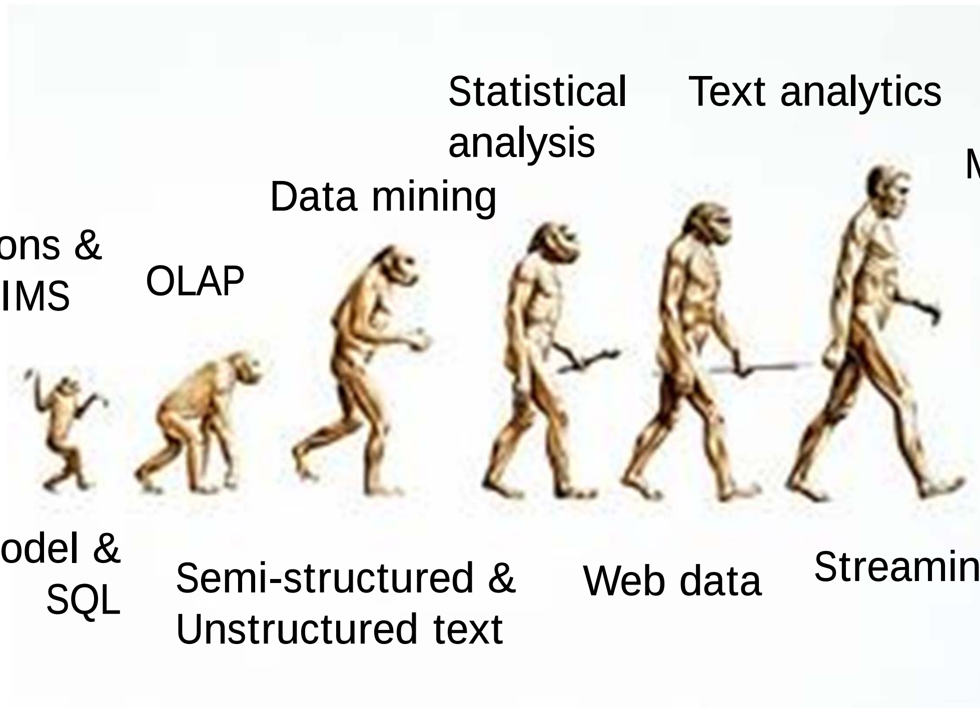
Model-Data Ecosystems:

Challenges, Tools, and Trends

Peter J. Haas
IBM Almaden Research Center



Great Progress in Analytics by the Database Community



Transactions & Reports, IMS

OLAP

Data mining

Statistical analysis

Text analytics

Machine learning

Massive Data/Cloud DB

Uncertain data

Relational model & SQL

Semi-structured & Unstructured text

Web data

Streaming data

Semantic data

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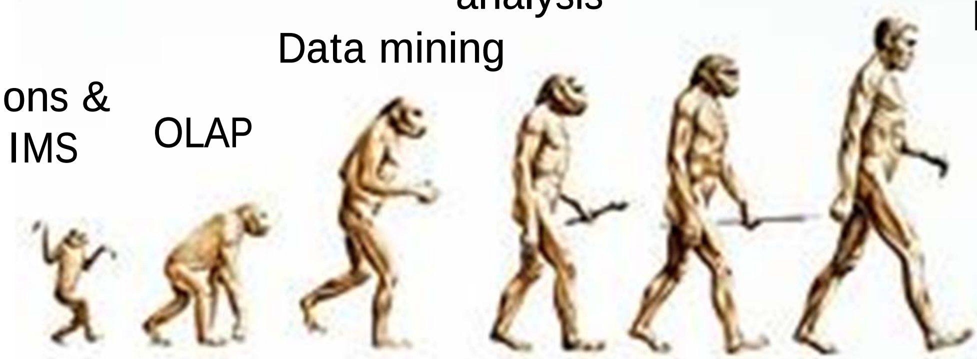

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BUT: Why do enterprises care about (big) data in the first place?

Because Enterprises Need to Make DECISIONS

informs online
Analytics Section

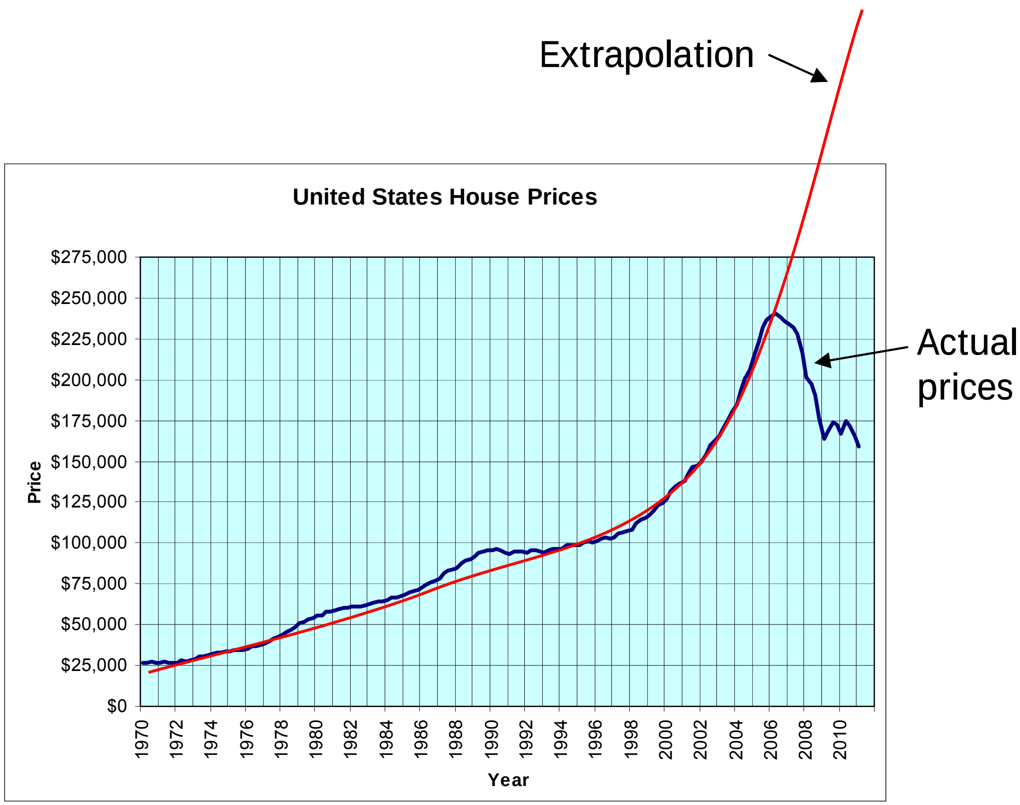
"Analytics is...a complete [enterprise] problem solving and decision making process"

Descriptive Analytics: Finding patterns and relationships in historical and existing data

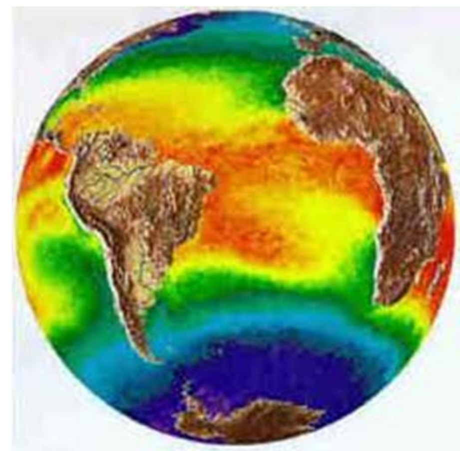
Predictive analytics: predict future probabilities and trends to allow what-if analysis

Prescriptive analytics: deterministic and stochastic optimization to support better decision making

Shallow Versus Deep Predictive Analytics



Extrapolation of 1970-2006 median U.S. housing prices



NCAR Community Atmosphere Model (CAM)

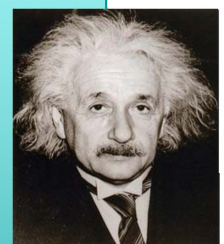
3.3 Eulerian Dynamical Core

$$
\begin{aligned}
\frac{\partial \zeta}{\partial t} &= \boldsymbol{k}\cdot\nabla\times(\boldsymbol{n}/\cos\phi) + F_{\zeta_H},\\
\frac{\partial \delta}{\partial t} &= \nabla\cdot(\boldsymbol{n}/\cos\phi) - \nabla^2(E+\Phi) + F_{\delta_H},\\
\frac{\partial T}{\partial t} &= \frac{-1}{a\cos^2\phi}\left[\frac{\partial}{\partial\lambda}(UT) + \cos\phi\frac{\partial}{\partial\phi}(VT)\right] + T\delta - \dot{\eta}\frac{\partial T}{\partial\eta} + \frac{R}{c_p^*}T_v\frac{\omega}{p}\\
&\quad + Q + F_{T_H} + F_{F_H},\\
\frac{\partial q}{\partial t} &= \frac{-1}{a\cos^2\phi}\left[\frac{\partial}{\partial\lambda}(Uq) + \cos\phi\frac{\partial}{\partial\phi}(Vq)\right] + q\delta - \dot{\eta}\frac{\partial q}{\partial\eta} + S,\\
\frac{\partial \pi}{\partial t} &= \int_1^{\eta_t}\boldsymbol{\nabla}\cdot\left(\frac{\partial p}{\partial\eta}\boldsymbol{V}\right)d\eta.
\end{aligned}
$$

Data is dead… Without What-If Models

Descriptive and shallow predictive analytics are **last resorts** for decision making in complex systems…

When you can't find the domain experts…



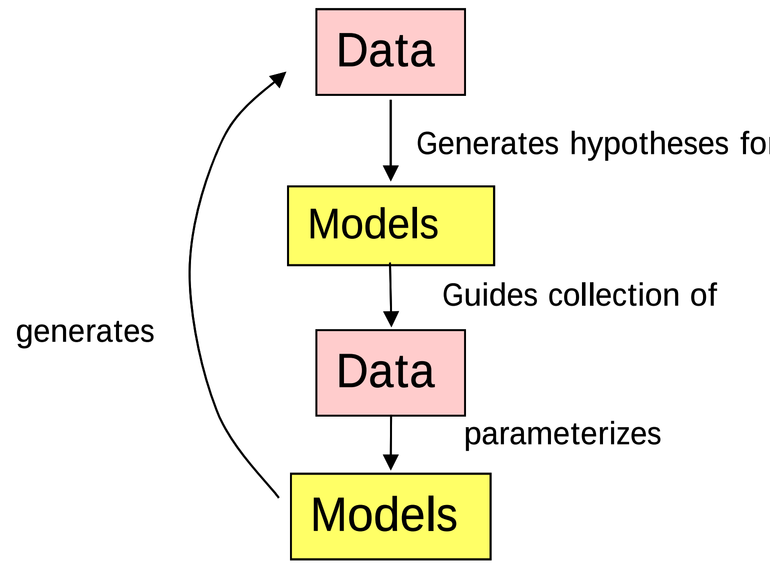
…but they are the main focus of most database and IM technology and research!

Need to supplement data with first-principles simulation models

- System structure
- Causal relationships
- Dynamics

…The notion that quantitative, numerical data are the only type of information needed to build an accurate model is flawed. In fact, I believe that the typical business obsession with numeric data can do more damage than good.

- Eric Bonabeau



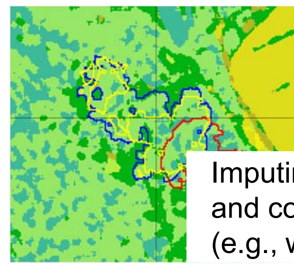
Ecosystem of Data and Models

Confluence of Research on (Big) Data Management & Predictive Analytics

Today: An idiosyncratic whirlwind tour of

Simulation and information integration

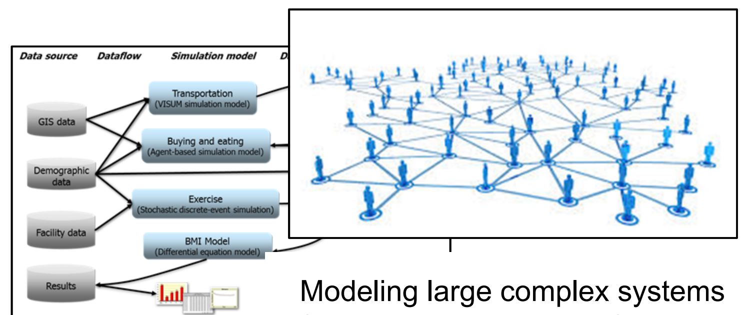
- Information integration via agent-based simulation
- Fusing real & simulated data (data assimilation)



Imputing missing data with models and correcting models with data (e.g., wildfire spread)

Data-intensive simulation

- Composite simulation models
  - Data transformation between models
  - Query optimization → simulation-run optimization
- Incorporating simulation into DB systems and vice versa



Modeling large complex systems (e.g., obesity, epidemics)

Goal: Some interesting examples to stimulate your thinking

π - shaped presentation, additional topics in paper (metamodeling)

Simulation and information integration

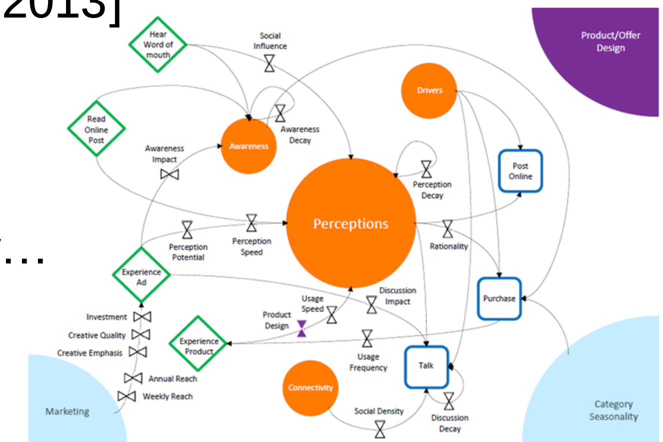
- Information integration via agent-based simulation
- Fusing real & simulated data (data assimilation)

Information Integration via Agent-Based Simulation

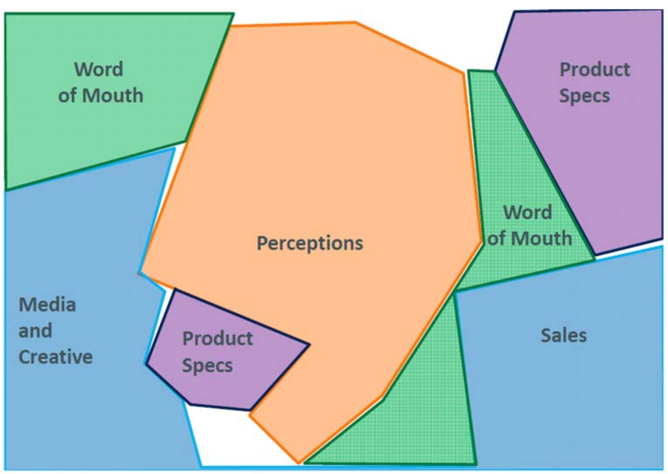
II via Agent-Based Simulation: Marketing Example

[Bonabeau, WSC 2013]

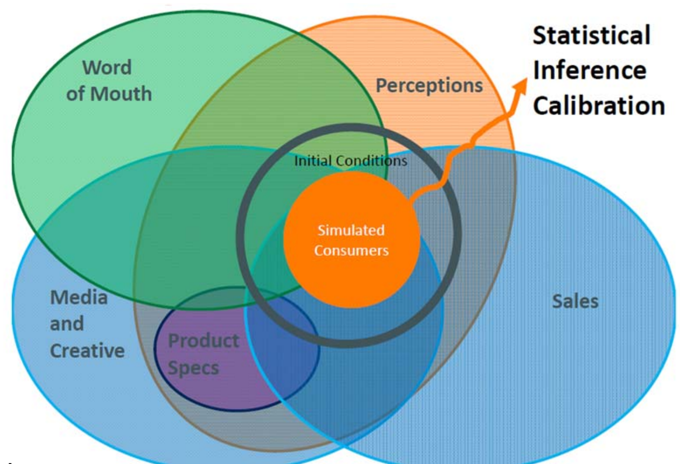
Many drivers of consumer behavior…



Non-overlapping datasets studied in isolation…



…are now integrated



Source: Eric Bonabeau

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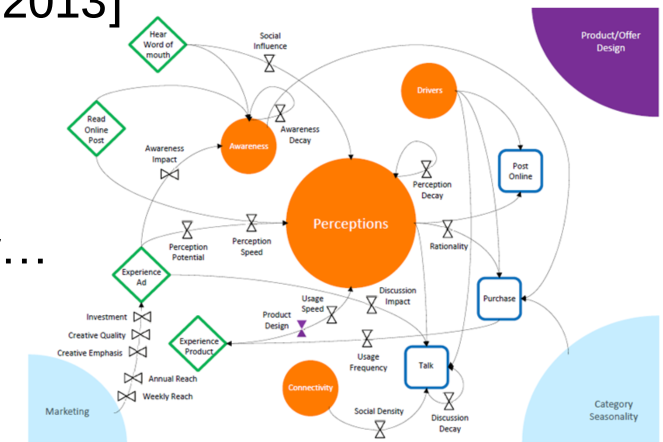
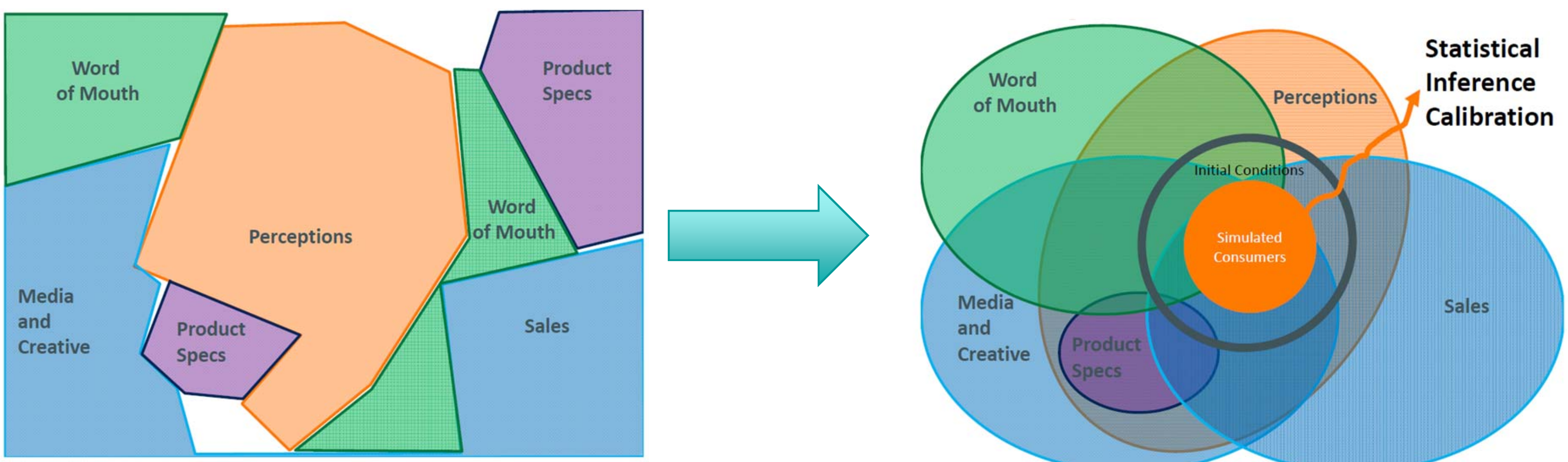


Key problem is model calibration (see paper)
- Maximum likelihood
- Method of simulated moments
- Machine learning?

Non-overlapping datasets studied in isolation…

…are now integrated



Source: Eric Bonabeau

Fusing Real and Simulated Data (Data Assimilation)

Fusing Real and Simulated Data: Data Assimilation

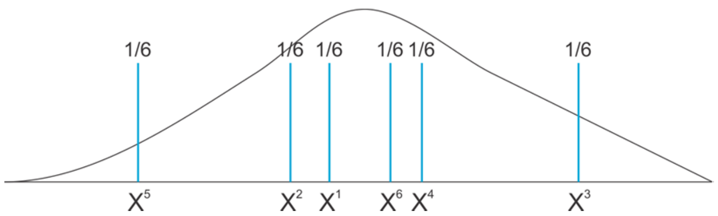
Integrate real and simulated data via particle filtering [Xue et al., 2012]

Classical Monte Carlo estimation of density $\pi_n(x_{1:n}) = \gamma_n(x_{1:n}) / Z_n$

$$\hat{\pi}_n(x_{1:n}) = \sum_{i=1}^{N} \frac{1}{N} \delta_{X^i_{1:n}}(x_{1:n}) \quad \text{so that}$$

$$\mathrm{E}[g(X_{1:n})] = \int g(x_{1:n}) \pi_n(x_{1:n})\, dx_{1:n}$$

$$\approx \int g(x_{1:n}) \hat{\pi}_n(x_{1:n})\, dx_{1:n} = \frac{1}{N} \sum_{i=1}^{N} g(X_{1:n})$$



- Can fail when n is large and/or π_n is complex (Z_n is often the culprit)

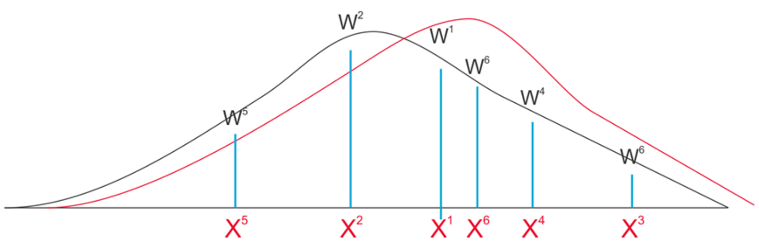
Importance sampling

- Sample from an "easier" importance density q_n and correct:

$$w_n(x_{1:n}) = \gamma_n(x_{1:n}) / q_n(x_{1:n})$$

$$\pi_n(x_{1:n}) = w_n(x_{1:n}) q_n(x_{1:n}) / Z_n \quad \text{and}$$

$$Z_n = \int w_n(x_{1:n}) q_n(x_{1:n})\, dx_{1:n}$$



- So draw N i.i.d. samples (particles) from q_n and insert MC approx. for q_n above:

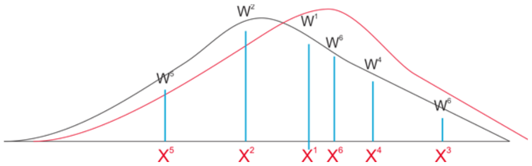
$$\hat{\pi}_n(x_{1:n}) = \sum_{i=1}^{N} W_N^i \delta_{X^i_{1:n}}(x_{1:n})$$

$$\text{where } W_N^i = w_n(X^i_{1:n}) / \sum_{j=1}^{N} w_n(X^j_{1:n})$$

Z_n not needed to compute weights

Data Assimilation, Continued

Sequential importance sampling (SIS)



- Importance sampling where $q_n(x_{1:n}) = q_1(x_1)\prod_{k=2}^{n} q_k(x_k \mid x_{1:k-1})$
- Recursive formula for weights:

$$w_n(x_{1:n}) = w_{n-1}(x_{1:n-1})\alpha(x_{1:n}) \text{ where } \alpha_n = \frac{\gamma_n(x_{1:n})}{\gamma_{n-1}(x_{1:n-1})q_n(x_n \mid x_{1:n-1})}$$

SIS with resampling (SISR)

- Stabilize SIS by resampling according to $W_n^1, W_n^2, \ldots, W_n^N$ at each step
- This is a sample from $\hat{\pi}_n$ --- set all new weights equal to $1/N$

{ (2, 0.7), (4, 0.2), (5, 0.1) }
→ { (2, 1/3), (2, 1/3) (5, 1/3) }

Particle filtering (SISR for hidden Markov models)

- Discrete time Markov chain $\{X_n\}_{n\geq 1}$ with transition probability density $p_n(x_n|x_{n-1})$
- Observation process $\{Y_n\}_{n\geq 1}$ with probs $p_n(y_n|x_n)$ of observation given true state
- Take $\gamma_n(x_{1:n}) = p_n(x_{1:n}, y_{1:n})$ so $\pi_n(x_{1:n}) = p_n(x_{1:n} \mid y_{1:n})$
- Optimal importance density (minimizes variance of weights):

$$q_n^*(x_n \mid x_{n-1}, y_{n-1}) \propto p_n(x_n \mid x_{n-1}) p_n(y_n \mid x_n)$$

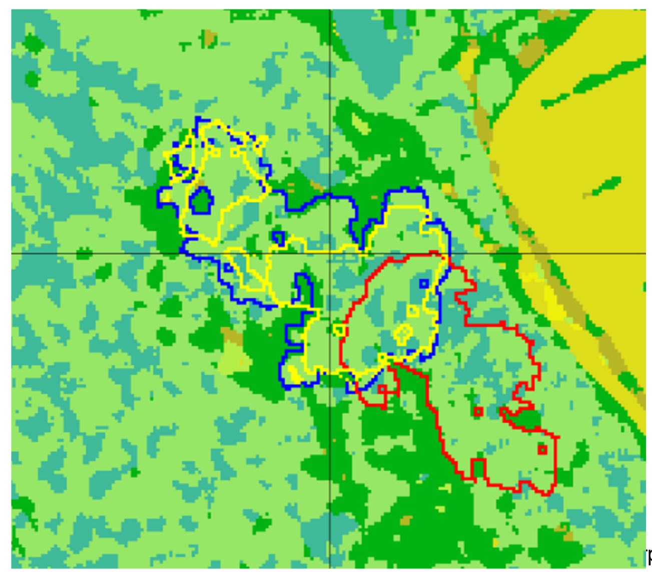
Data Assimilation, Continued

Application to data assimilation [Xue et al., 2013]

- DEVS-FIRE model
  - Models stochastic progression of wildfire over gridded terrain
  - State $\in$ {unburned, burned, burning-intensity}
  - Merge model data x and sensor data y: $p_n(x_n|y_n)$
- Gaussian sensor model: $p_n(y_n|x_n)$
- Original importance density: $p_n(x_n|x_{n-1})$, $n>1$
  - To sample from importance density (step 6), run simulation for 1 time step
  - Analytical expressions (step 8) reduce to sensor model
  - Ignores sensor reading
    recall: $q_n^*(x_n \mid x_{n-1}, y_{n-1}) \propto p_n(x_n \mid x_{n-1}) p_n(y_n \mid x_n)$
- Improved sensor-aware importance density under development
  - Model and sensors weighted according to "confidence"
  - Kernel density estimation used to obtain analytical expressions (step 8)

Algorithm 2 Particle Filtering

1: Sample $\{X_1^i\}_{1\le i\le N}$ from $q_1(x_1 \mid Y_1)$
2: Compute weights $w_1(X_1^i) = p_1(X_1^i) p_n(Y_1 \mid X_1^i)/q_n(X_1^i \mid Y_1)$ for $1 \le i \le N$
3: Compute normalized weights $\{W_1^i\}_{1\le i\le N}$
4: Resample $\{(W_1^i, X_1^i)\}_{1\le i\le N}$ to obtain $\{(\frac{1}{N}, \bar{X}_1^i)\}_{1\le i\le N}$
5: **for** $n \ge 2$ **do**
6: Sample $\{X_n^i\}_{1\le i\le N}$ from $q_n(x_n \mid Y_n, \bar{X}_{n-1}^i)$
7: **for** $i = 1, 2, \ldots, N$ **do**
8: Compute weight $\alpha_n^i = p_n(Y_n \mid X_n^i) p_n(X_n^i \mid \bar{X}_{n-1}^i)/q_n(X_n^i \mid Y_n, \bar{X}_{n-1}^i)$
9: **end for**
10: Compute normalized weights $W_n^i = \alpha_n^i / \sum_{j=1}^N \alpha_n^j$ for $1 \le i \le N$
11: Resample $\{(W_n^i, X_n^i)\}_{1\le i\le N}$ to obtain $\{(\frac{1}{N}, \bar{X}_n^i)\}_{1\le i\le N}$
12: **end for**



Data-intensive simulation

- Composite simulation models
  - Data transformation between models
  - Query optimization → simulation-run optimization
- Incorporating simulation into DB systems and vice versa

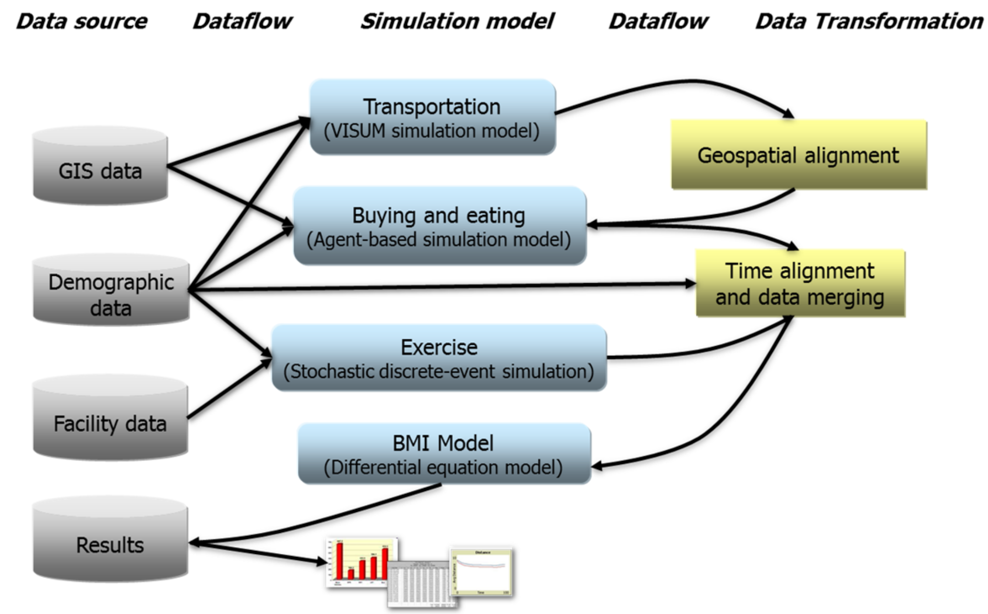
Composite Simulation Models

Composite Simulation Models: Overview

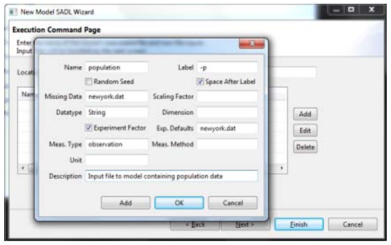
- Motivation:
  - Domain experts have different worldviews
  - Use different vocabularies
  - Sit in different organizations
  - Develop models on different platforms
  - Don't want to rewrite existing models!

- Composite modeling approach
  - Combines data integration with simulation
  - Loose coupling via data exchange
  - Metadata for detection and semi-automatic correction of data mismatches
  - Ex: Splash prototype [Tan et al., IHI 2012]

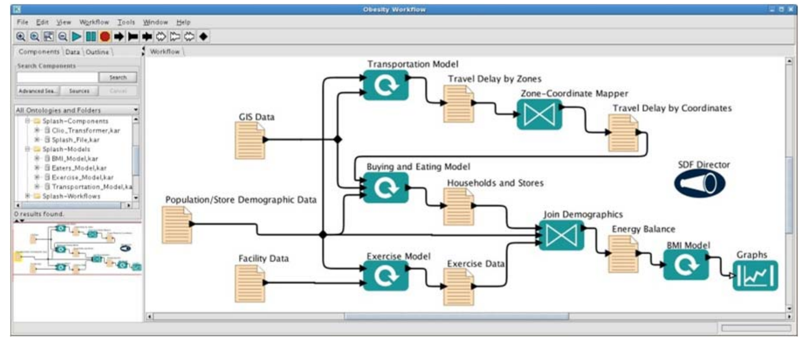
- Advantages
  - Model curation and re-use
  - Flexibility
  - No need for "universal" platform, API, etc.



Composite Simulation Models: Splash Example

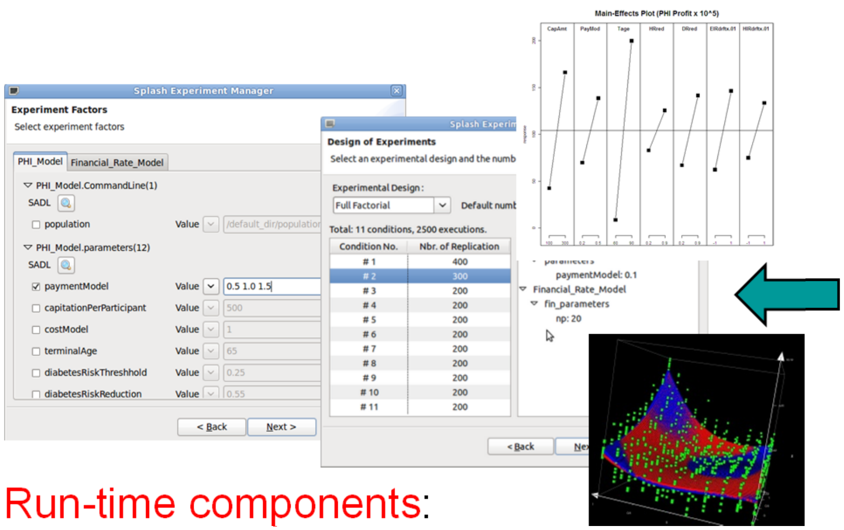


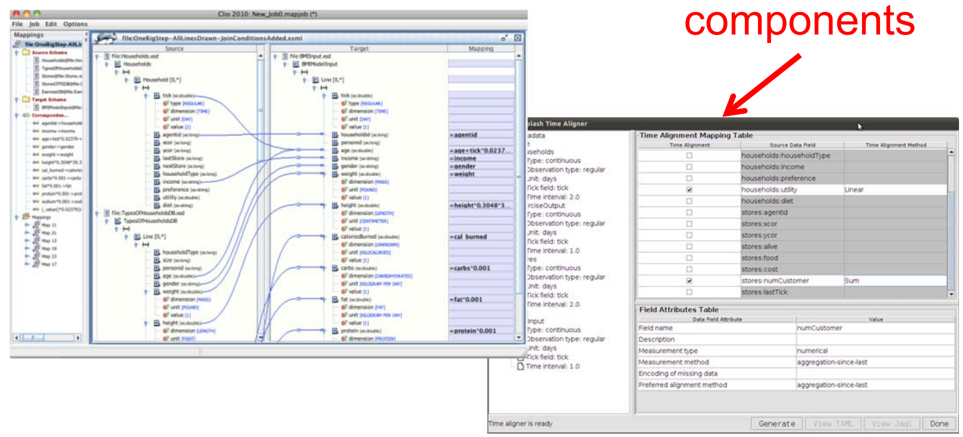
SADL metadata language



Kepler adapted for model composition

Design-time components





Run-time components:

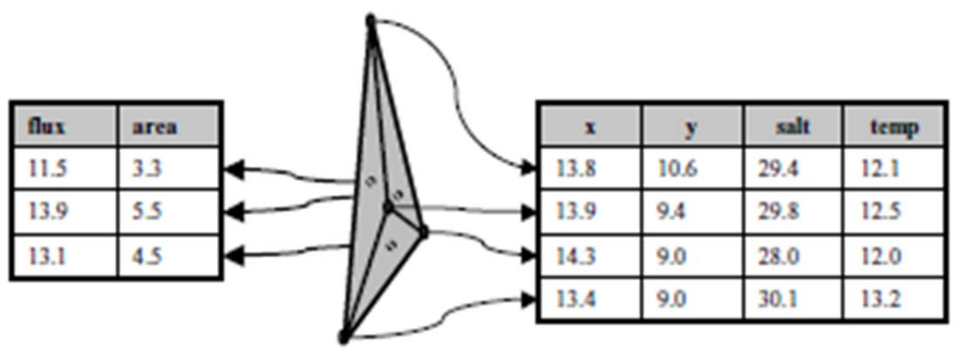
- Kepler adapted for model execution
- Experiment Manager
  (sensitivity analysis, metamodeling, optimization)

Data transformation tools:

- Clio++
- Time Aligner (MapReduce algorithms)
- Templating mechanism

Composite Simulation Models: Data transformation I

- Algebra of “gridfields” [Howe and Maier, VLDBJ 2005]
  - Grid: collection of cells (of various dimension) + incidence relation
    - x ≼ y if
      - dim(x) = dim(y) and x = y; or
      - dim(x) < dim(y) and x “touches” y
  - Gridfield = grid + mappings from cells to data values
  - Key operation on gridfields: regrid
    - Maps set S of source cells to a given target cell
    - Applies aggregation functions to S to compute associated data values
  - Restrictions (a kind of selection) commute with regrid → optimizations



Source: Howe & Maier

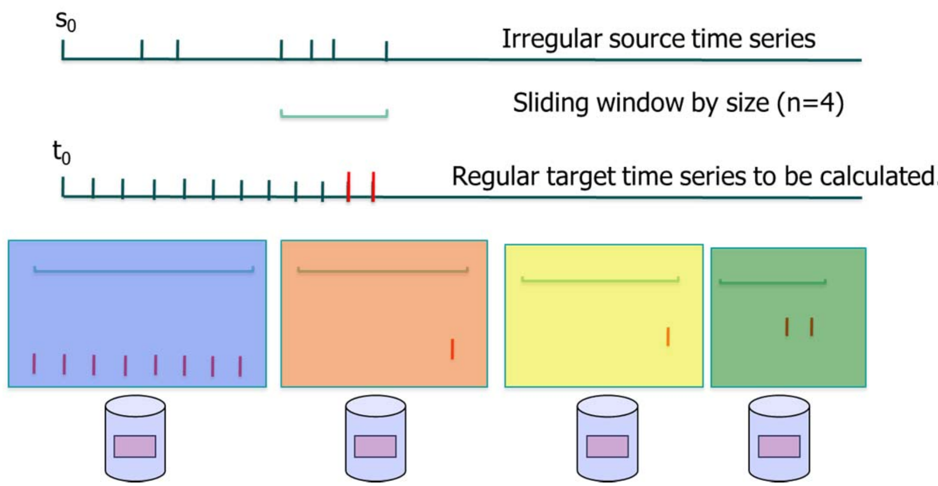
Fig. 1 Datasets bound to the nodes and polygons of a 2-D grid

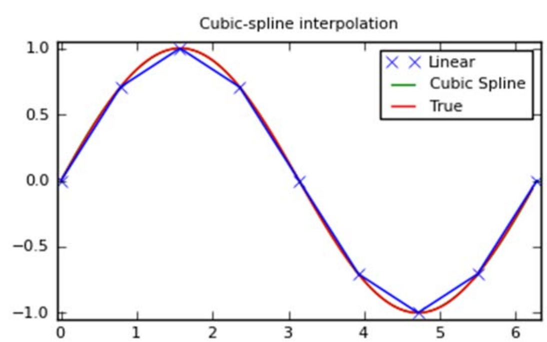
Composite Simulation Models: Data Transformation II

Massive scale time alignment

- Common Splash time alignment operation:

  Interpolating (massive) time-series data
- Parallelize on Hadoop
- Linear interpolation: easy
- Cubic spline interpolation: hard
  - Computing spline constants = solving massive tri-diagonal linear system
  - Solution: distributed stochastic gradient descent algorithm (see paper)



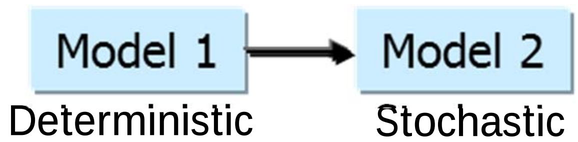


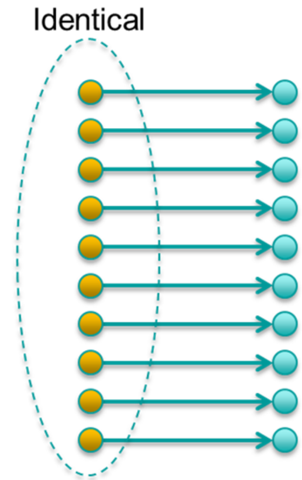
$$A = \begin{pmatrix} \frac{h_0+h_1}{3} & \frac{h_1}{6} & 0 & \cdots & 0 & 0 & 0 \\ \frac{h_1}{6} & \frac{h_1+h_2}{3} & \frac{h_2}{6} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{h_{m-3}}{6} & \frac{h_{m-3}+h_{m-2}}{3} & \frac{h_{m-2}}{6} \\ 0 & 0 & 0 & \cdots & 0 & \frac{h_{m-2}}{6} & \frac{h_{m-2}+h_{m-1}}{3} \end{pmatrix} \quad b = \begin{pmatrix} \frac{d_2-d_1}{h_1} - \frac{d_1-d_0}{h_0} \\ \frac{d_3-d_2}{h_2} - \frac{d_2-d_1}{h_1} \\ \vdots \\ \frac{d_m-d_{m-1}}{h_{m-1}} - \frac{d_{m-1}-d_{m-2}}{h_{m-2}} \end{pmatrix}$$

Solve: Ax = b

Composite Simulation Models: Optimizing Simulation Runs

Motivating example: Two models in series, 100 reps

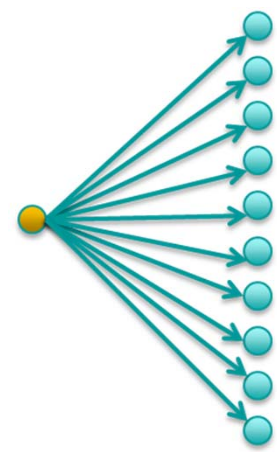




- Naïve approach: execute composite model (i.e., Models 1 & 2) 100 times

- A better approach:

  - Execute Model 1 once and cache result
  - Read from cache when executing Model 1

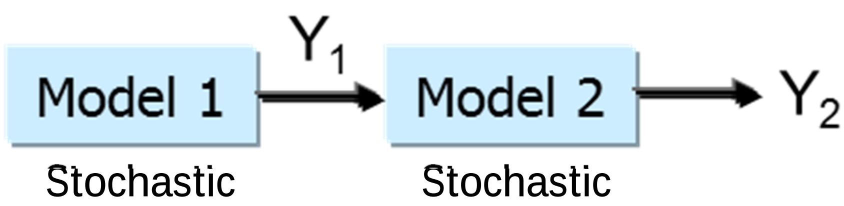


Question: Can result-caching idea be generalized?

Optimizing Simulation Runs (Continued)

Result-Caching: General Method for Two Models [Haas, WSC 2014]

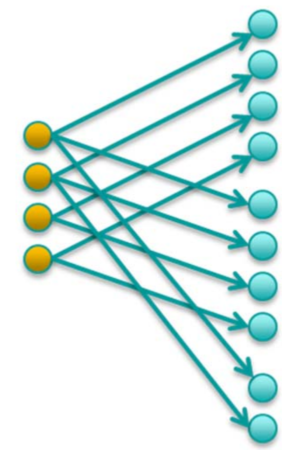
- Running example: Two models in series



- Goal: Estimate $\theta = E[Y_2]$ based on n replications

- Result-caching approach:

  1. Choose $\alpha \in (0,1]$ (the re-use factor)
  2. Generate $\lceil \alpha n \rceil$ outputs from Model 1 and cache them
  3. To execute Model 2, cycle through results
  4. Estimate θ by $\theta_n = n^{-1} \sum_{i=1}^{n} Y_{2;i}$ ← Dependent



Ex: n=10, $\lceil \alpha n \rceil = 4$

Result-Caching: Optimizing the Re-Use Factor

Budget-constrained setting [Glynn & Whitt 1992]

- Cost of producing n outputs from Model 2 is $C_n = \sum_{j=1}^{\lceil \alpha n \rceil} \tau_{1;j} + \sum_{j=1}^{n} \tau_{2;j}$ (random)
- Under (large) fixed computational budget c:
  - Number of Model 2 outputs produced is $N(c) = \max\{n \geq 0 : C_n \leq c\}$
  - Estimator is $U(c) = \theta_{N(c)}$ (average of a random # of dependent variables)

Key result: a central limit theorem

Suppose that $E[\tau_1 + \tau_2 + Y_2^2] < \infty$. Then U(c) is asymptotically $N(\theta, g(\alpha)/c)$.

where $r_\alpha = \lfloor 1/\alpha \rfloor$ and

$$g(\alpha) = (\alpha E[\tau_1] + E[\tau_2])\left\{Var[Y_2] + \left(2r_\alpha - \alpha r_\alpha (r_\alpha + 1)\right) Cov[Y_2, Y_2']\right\}$$

(expected cost per obs.) x (variance per obs.)

- Thus, minimize $g(\alpha)$ [or maximize asymptotic efficiency = $1/g(\alpha)$]

Result-Caching: The Optimal Re-Use Factor

Optimal solution

- Assume that $Cov[Y_2, Y_2'] \geq 0$
- Approximate r_α by $1 / \alpha$

$$\alpha^* \approx \left(\frac{E[\tau_2] / E[\tau_1]}{\left(Var[Y_2] / Cov[Y_2, Y_2']\right) - 1} \right)^{1/2} \wedge \quad 1$$

Observations

- If Model 1 cost is large relative to Model 2, then high re-use of output
- If Model 2 insensitive to Model 1 (Cov << Var), then high re-use
- If Model 1 is deterministic (Cov = 0), then total re-use

Ongoing work

- Generalize to > 2 models (math similar to sampling-based join-size estimation)
- Develop techniques to compute/approximate needed statistics
- In general: Extend query optimization to “simulation-run optimization”

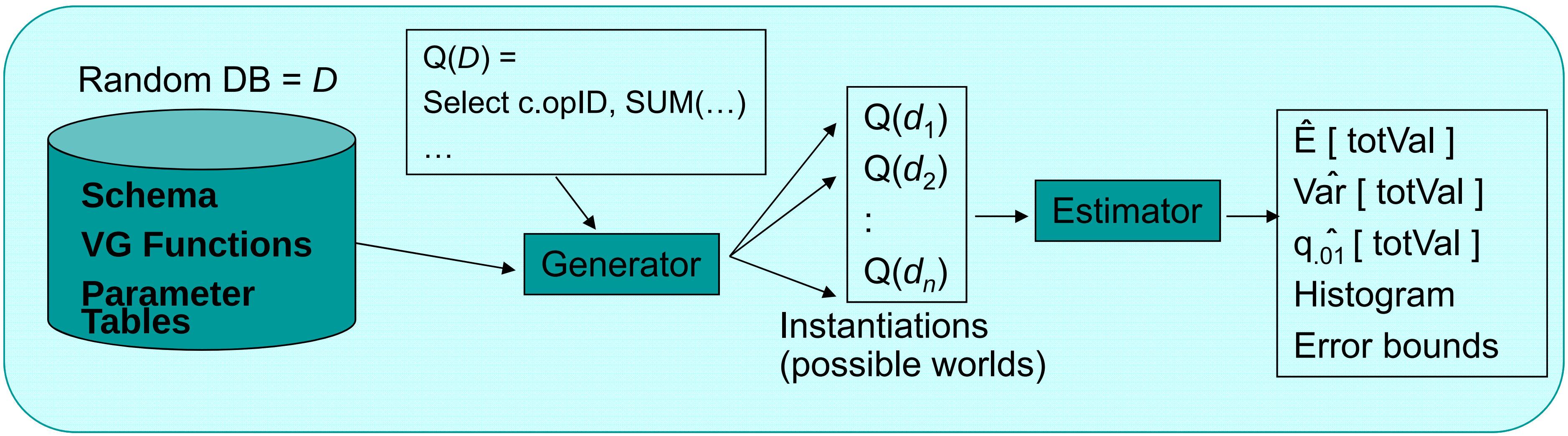
Incorporating Simulation into DB Systems

Incorporating Simulation into DB I: MCDB [Jampani et al., TODS 2011]

```
CREATE TABLE optionVal (opID, val) AS
  FOR EACH o IN option
    WITH oVal AS optionSim(
       VALUES(o.initVal, o.r, o.sigma, o.k, o.m, o.T))
SELECT o.opID, v.VALUE FROM oVal v
```

← Stochastic table

optionSim = Value generation (VG) function



- Implementation uses “tuple bundle” techniques, parallel DB & MapReduce execution
- Challenges: extreme quantiles, threshold queries (>2% decline in sales with prob > 50%)

Incorporating Simulation into DB II: SimSQL

- Re-implementation and extension of MCDB [Cai et al., SIGMOD 2013]
  - Database sequence: D[0], D[1], D[2], ...
  - VG function for D[i] can be parameterized on **any** table in D[i-1]
  - I.e., Can simulate database-valued Markov chains

- Potential application to massive-scale agent-based simulations [Wang et al., VLDB, 2010]

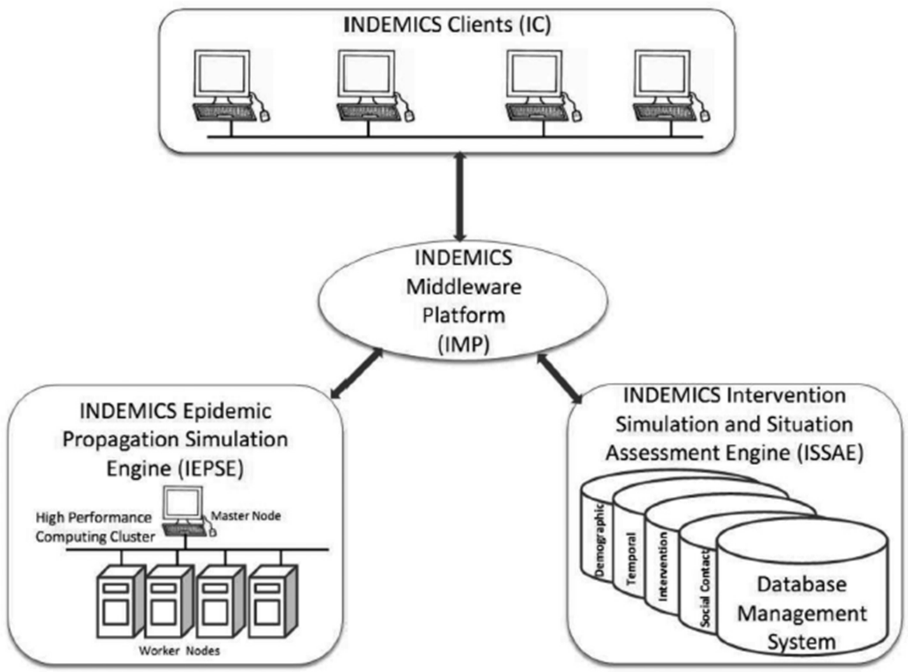
ID	LocX	LocY	DState	Vaccinated?	...
agent1	2.34	2.48	Infected	N	...
agent2	3.57	3.72	recovered	N	...
agent3	50.20	80.9	susceptible	Y	...

- Agent-based simulation = sequence of self-joins
  - Often, only nearby agents interact, so can exploit parallel processing
  - Not really explored in SimSQL setting

Incorporating DB Systems into Simulation

Incorporating DB into Simulation: Indemics

- Indemics system for simulating epidemics [Bisset et al., ACM TOMACS 2014]
  - Uses HPC for compute-intensive tasks (disease propagation), DBMS for data-intensive tasks (state assessment and intervention)
  - Observer can stop simulation, input an intervention, then resume



Source: Bisset et al.

Network epidemic model

Database of demographic info

Indemics, Continued

Example intervention strategy:

Algorithm 1 Vaccinate preschoolers if more than 1% are sick

```
CREATE TABLE Preschool(pid) AS
  (SELECT pid FROM Person WHERE 0 ≤ age ≤ 4);
/* Based on demographic data */
DEFINE nPreschool AS (SELECT COUNT(pid) FROM Preschool);
for day = 1 to 300 do
    /* Based on demographic and disease dynamic data */
    WITH InfectedPreschool (pid) AS
     (SELECT pid FROM Preschool, InfectedPerson
      WHERE Preschool.pid = InfectedPerson.pid);
    DEFINE nInfectedPreschool AS
     (SELECT COUNT(pid) FROM InfectedPreschool);
    if nInfectedPreschool > 1% × nPreschool then
        Apply vaccines to SELECT( pid FROM Preschool);
        /* Intervention subpopulation and action */
    end if
end for
```

Formal model of system:

- Coevolving Graphical Discrete Dynamical System (CGDDS)
- Partially observable Markov decision process (POMDP)

Conclusions

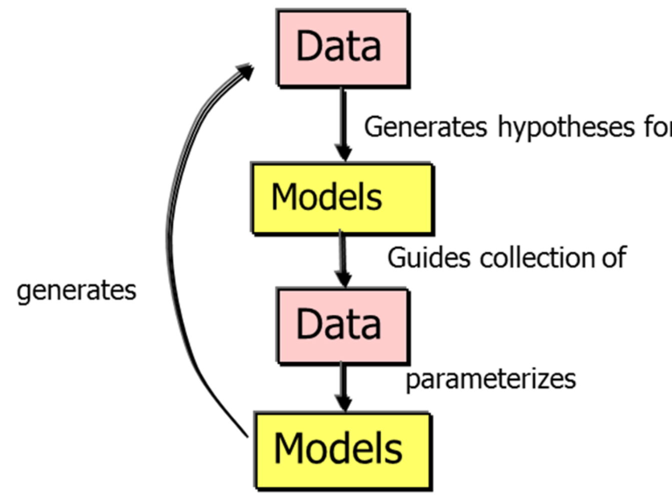
- Intertwining of data management and simulation — both are needed
- Many problems in early stages, need formalization
- Lots of room for interesting research!

Data-intensive simulation

- Composite simulation models
  - Data transformation between models
  - Query optimization → simulation-run optimization
- Incorporating simulation into DB systems and vice versa

Simulation and information integration

- Information integration via agent-based simulation
- Fusing real & simulated data (data assimilation)



Ecosystem of Data and Models

IBM Research

Model-Data Ecosystems:

Challenges, Tools, and Trends

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