Morphisms: Exact and Approximate

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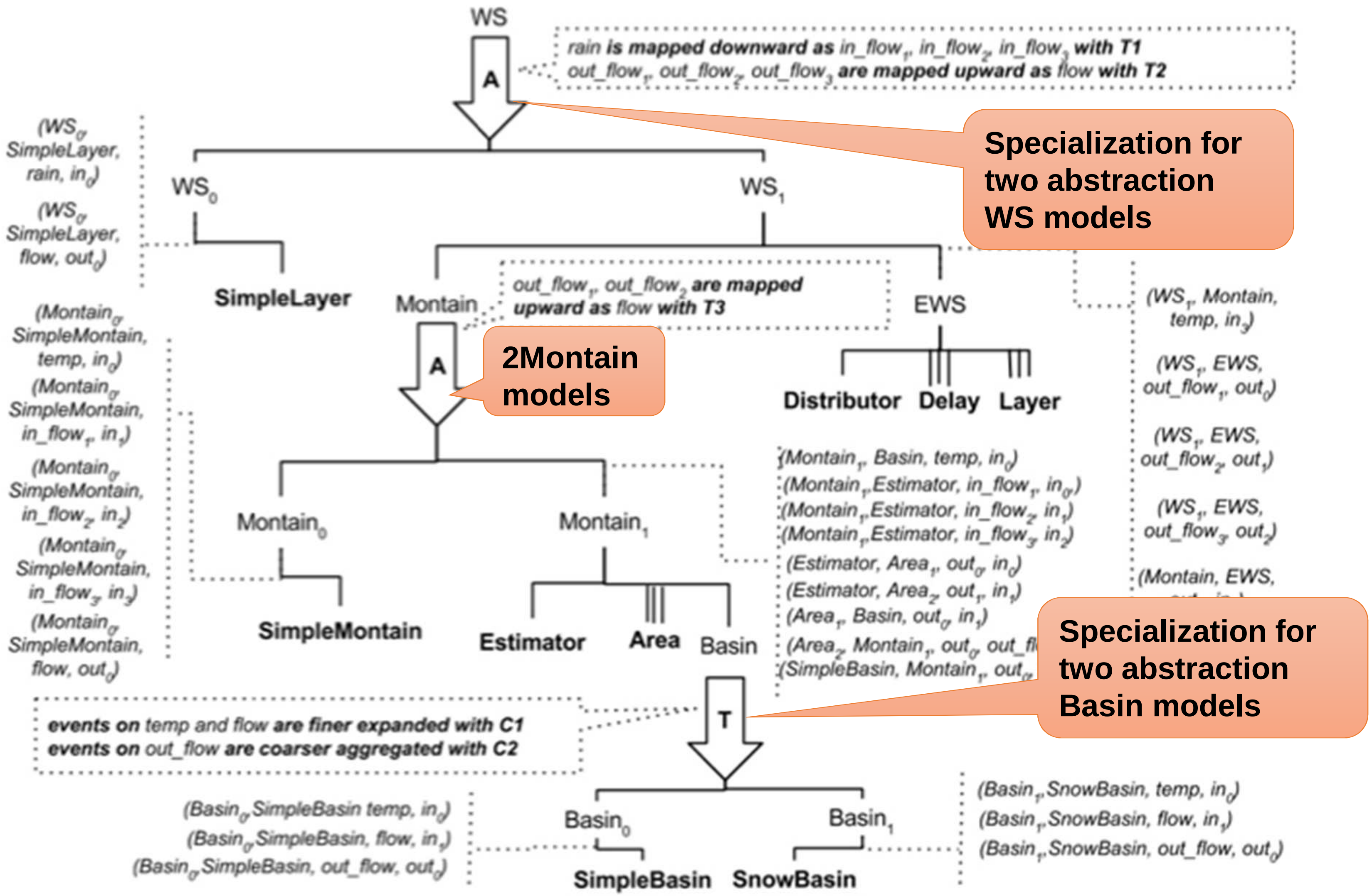
Outline

- **The need to consider multi-level model approximation families**
- **Some background theory – dynamic systems and morphisms provide a mathematical basis**
- **Some sufficient conditions that enable exact approximation**
- **Approximate Morphisms to handle departures from enabling conditions**
- **Error propagation and example of sensitivity analysis**
- **Construction of multi-level model approximation families**

The need to consider multi-level model approximation families

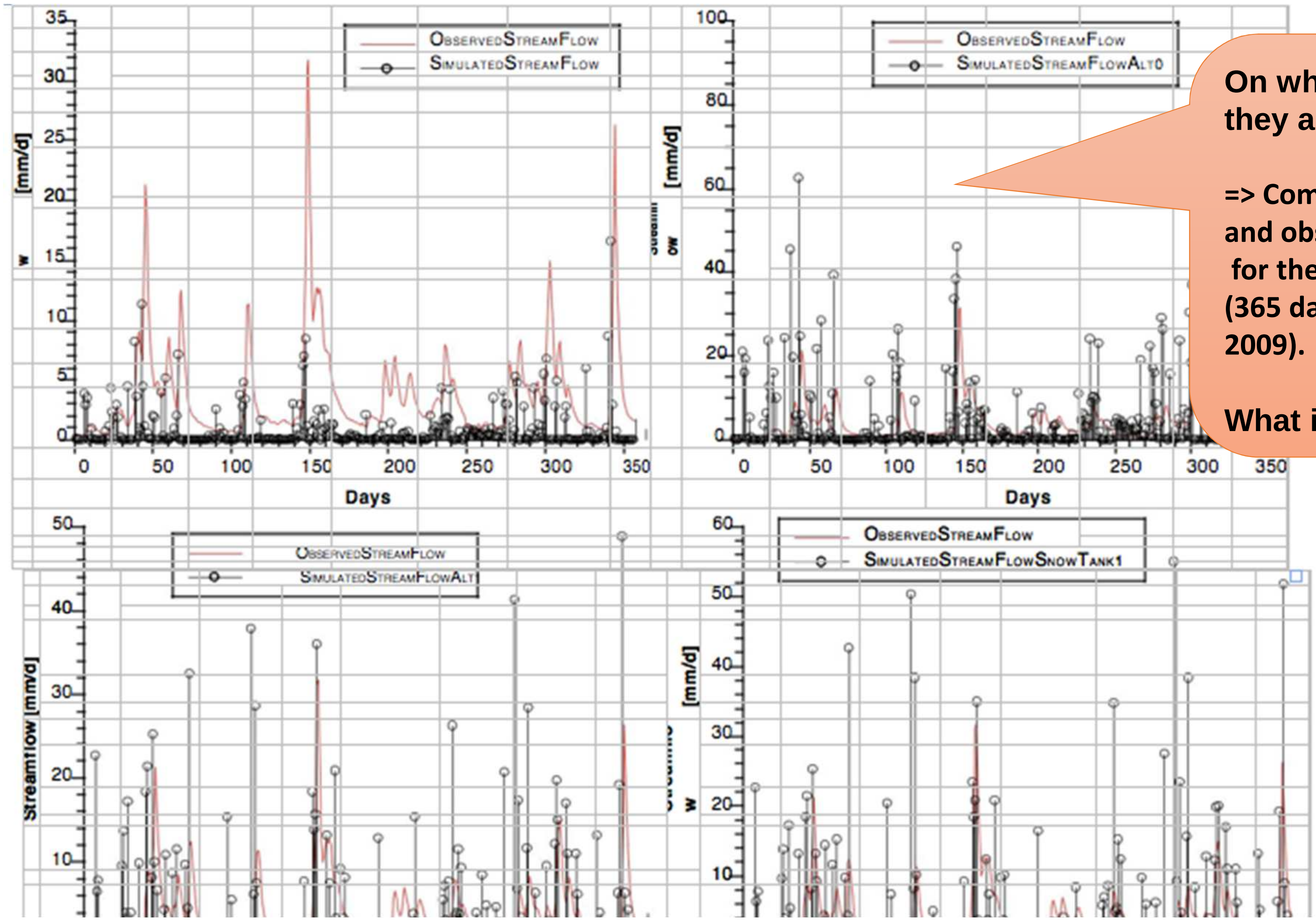
- Systems of Systems (SoS) may be modeled at different levels of spatial extent and resolution (municipal, county, state…)
- Models may be constructed at coarse abstraction levels that support faster simulation - e.g., model checking – but not Pacman
- Models may be constructed at high fidelity that are purported to be closer to reality, but how well do we know the details
- How can we ensure that errors introduced in the aggregation/disaggregation processes lie within acceptable limits?
- Interoperation of models at different levels of resolution presupposes effective ways to develop and correlate the underlying abstractions
- An useful methodology for integrated family of approximation models would allow
  - flexibility in calibration and cross-calibration
  - application to diverse experimental frames, i.e. properties

Implementation: Case Study: A Watershed behavior



Implementation: Results

Results of simulation of 4 pruned and transformed compositions: Each figure presents a time series



On what basis should they agree?

=> Comparing simulated and observed daily flows for the one-year period (365 days for the year 2009).

What if they disagree?

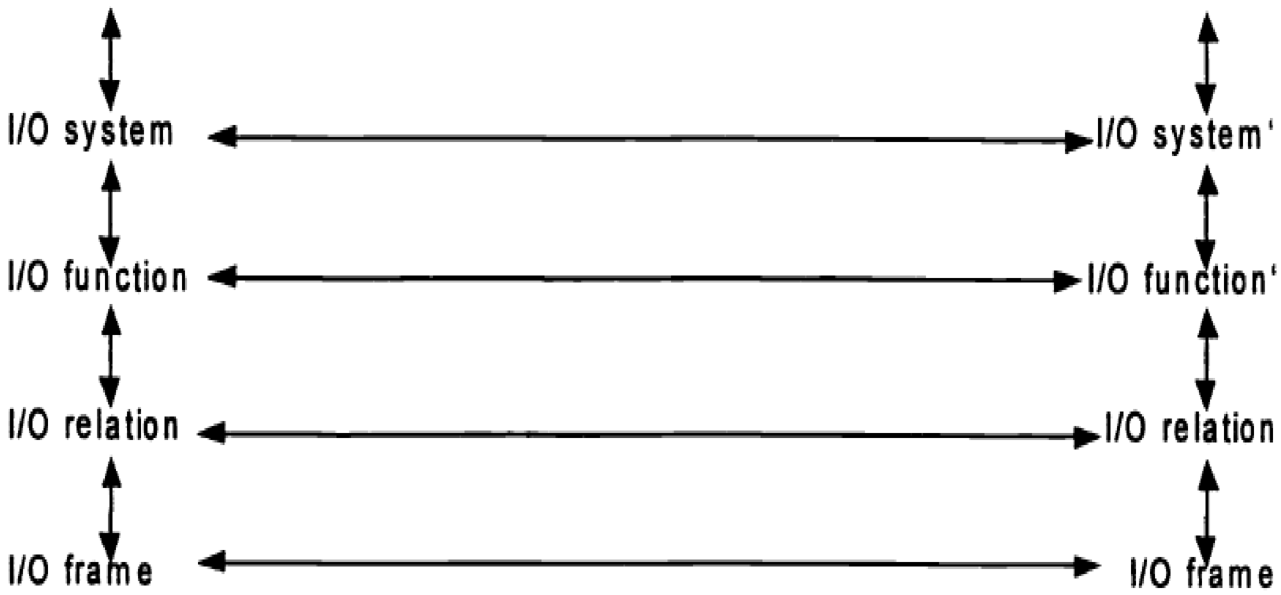
Some background theory – dynamic systems and morphisms provide a mathematical basis

- Systems theory generalizes finite state and linear theory exact and approximate model approximation
- Framework for M&S provides needed concepts for approximate model construction, including model-simulator separation and experimental frames
- Systems theory provides morphism concepts for exact model simplification
- M&S Framework enables System morphism concepts to be extended to handle approximate model construction and error propagation analysis

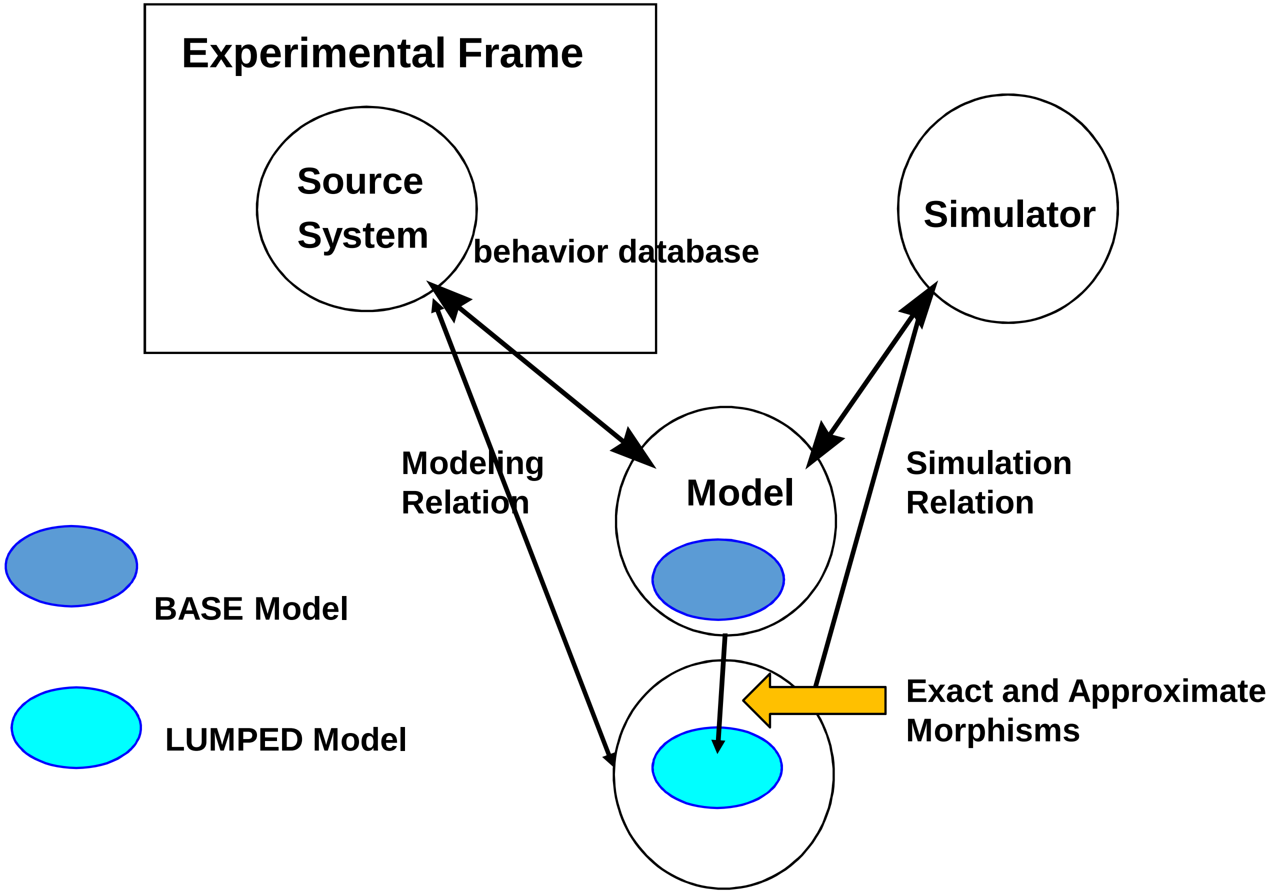
Stratification of System Knowledge/Specification Levels

Level	Specification Name	Two Systems are Morphical at this level if:
0	Observation Frame	their inputs, outputs and time bases can be put into correspondence
1	I/O Behavior	they are morphic at level 0 and the time-indexed input/output pairs constituting their I/O behaviors also match up in one-one fashion
2	I/O Function	they are morphic at level 0 and their initial states can be placed into correspondence so that the I/0 functions associated with corresponding states are the same
3	I/O System	the systems are homomorphic (explained below)

Associated Structure/Behavior Preserving Morphisms



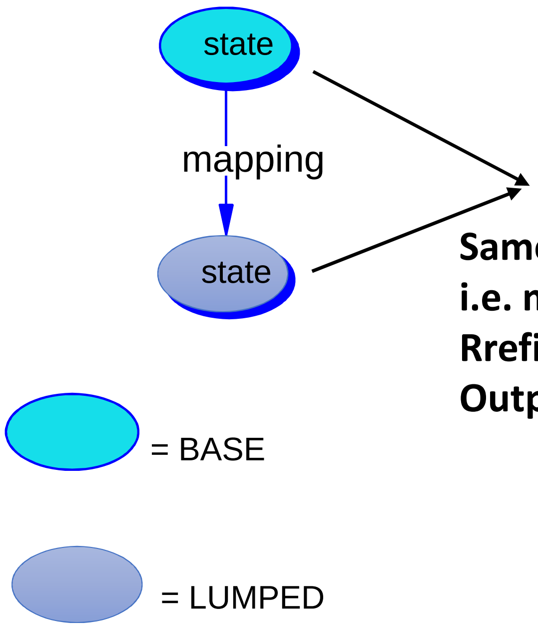
Modeling and Simulation Framework



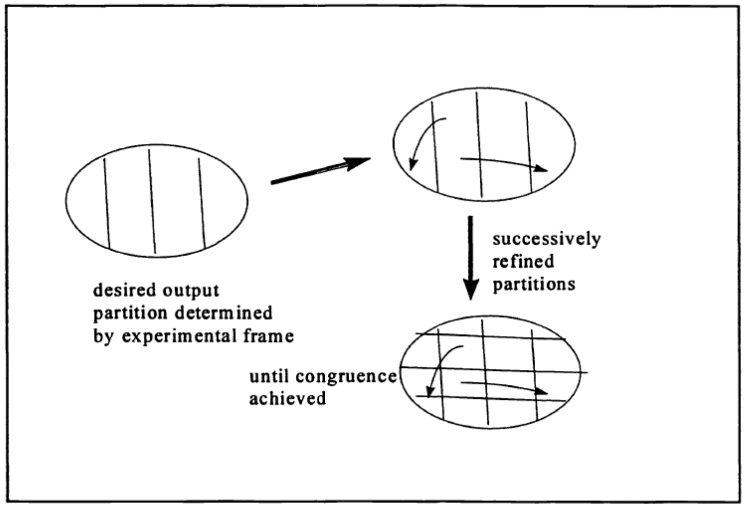
Abstraction is defined as valid model simplification and is relative to one or more experimental frames

[PLOS Computational Biology: Minimum Information About a Simulation Experiment (MIASE)]

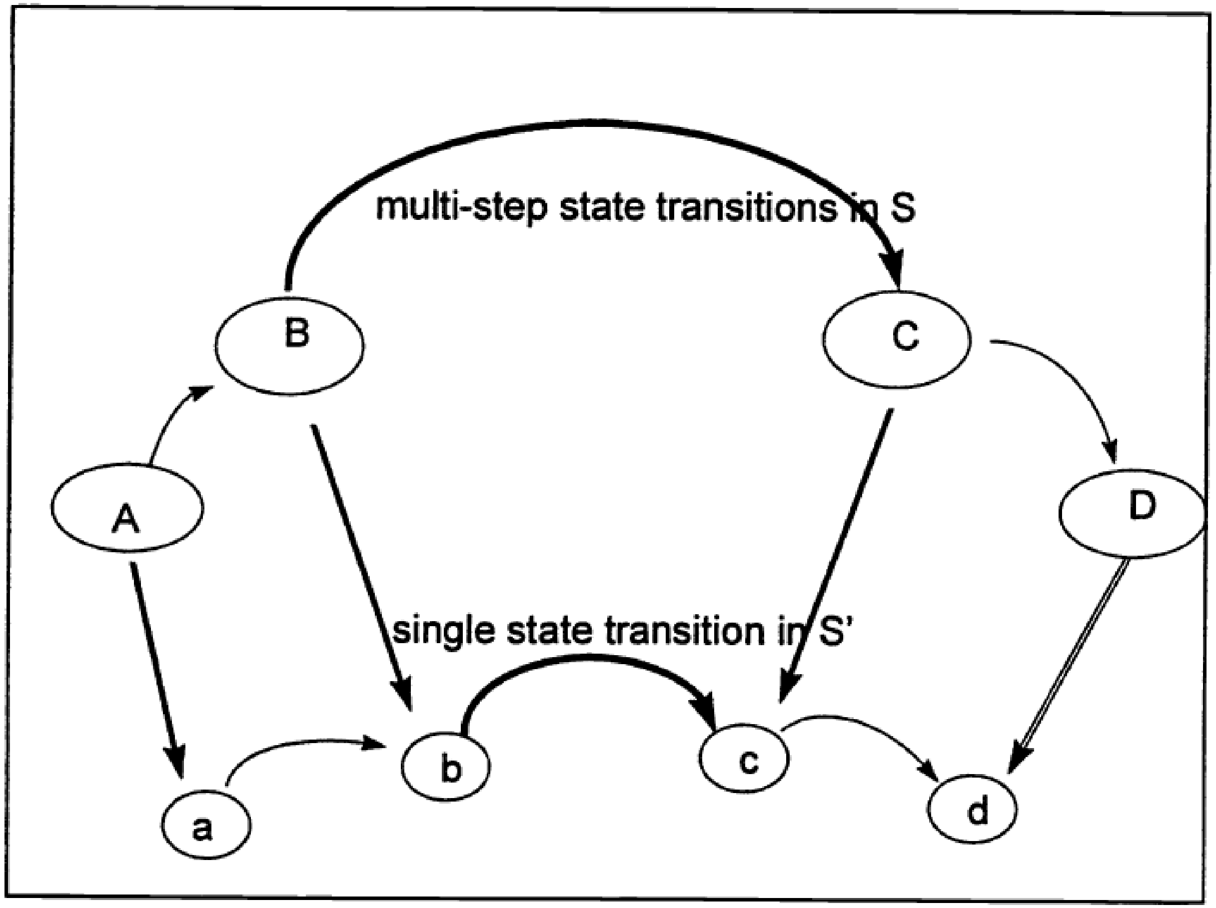
Experimental Frames Determine Validity of Abstraction



Same output
i.e. mapping
Rrefines the
Output partition



Multi-step morphism allows micro states and input/output encoding/decoding



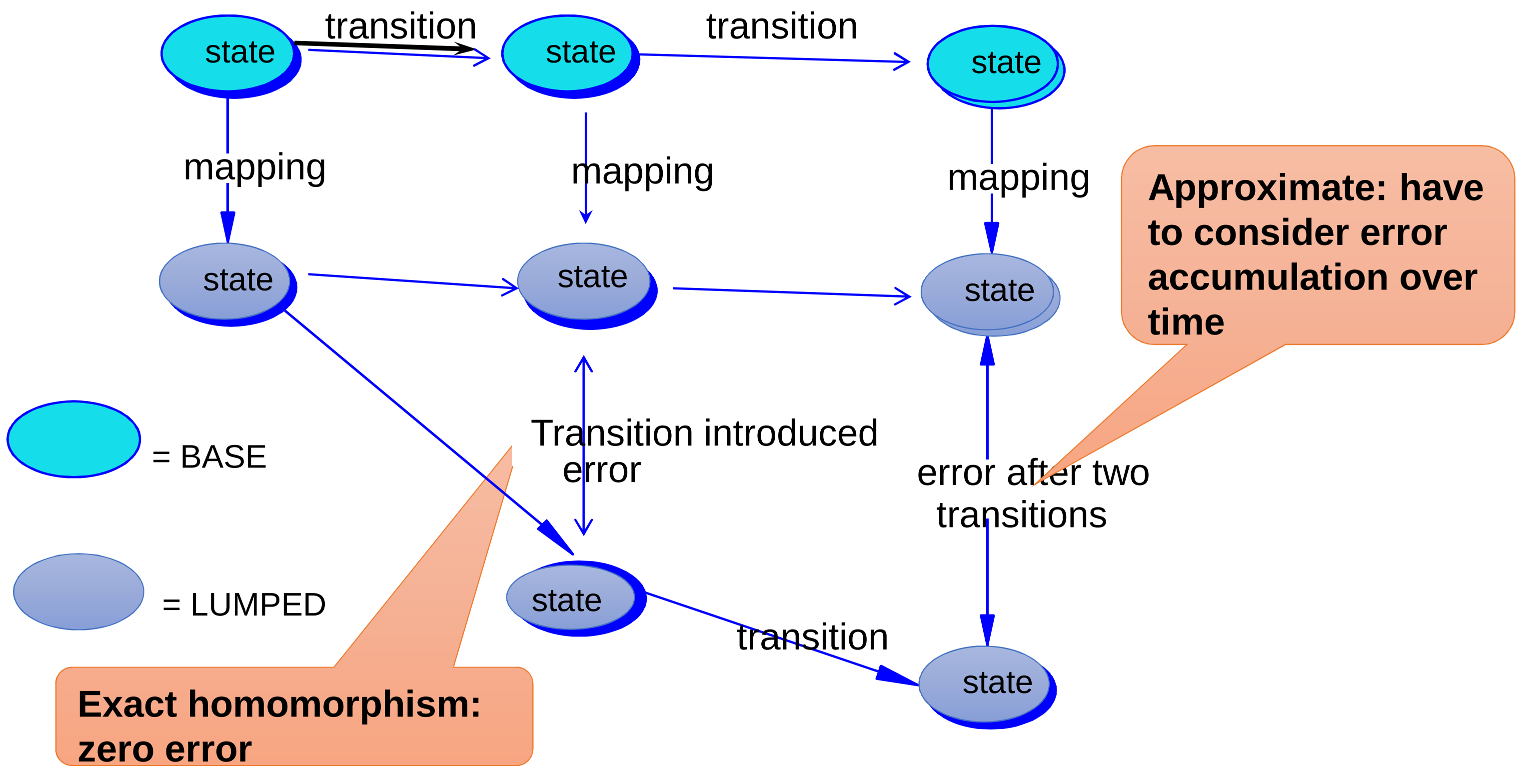
Some sufficient conditions that enable exact abstraction

- Finite state theory provides algorithms employing congruence relations, state set partitions, and output refinement
- Linear systems theory developed model realization theory that was shown to be essentially equivalent to finite state theory
- Probabilistic automata provided somewhat different lumpability criteria
- These concepts were generalized in dynamic system theory within the M&S framework

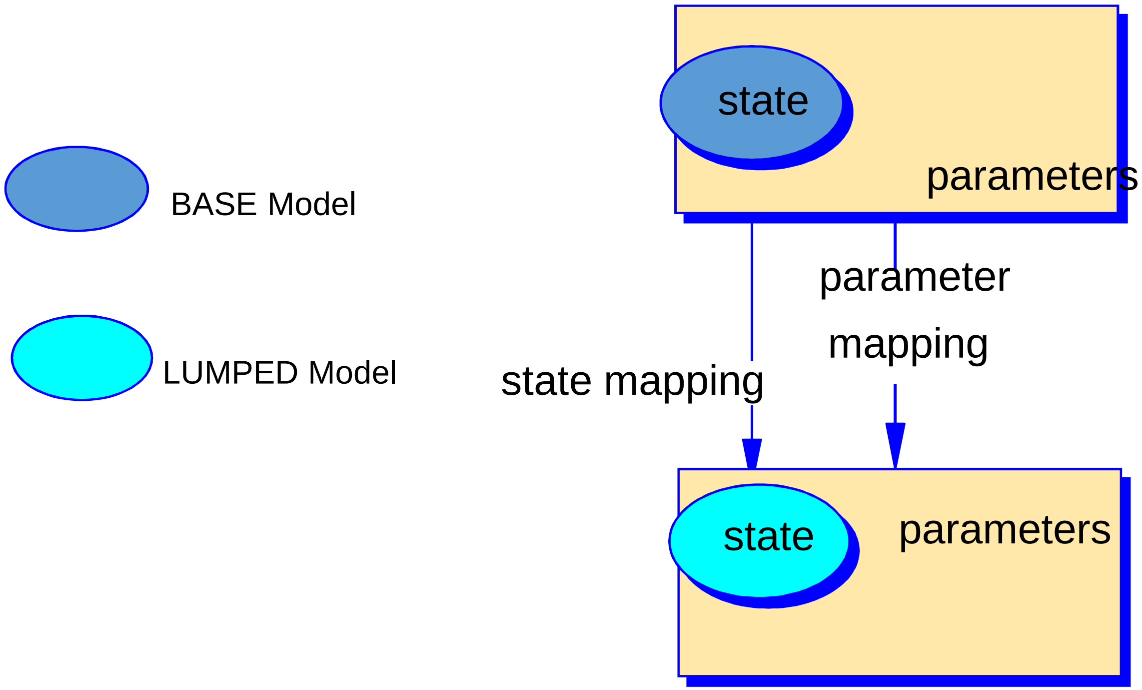
State system homomorphism: exact and approximate

Homomorphism concepts borrowed from finite state automata

require base and lumped model states to **remain in state correspondence over time**

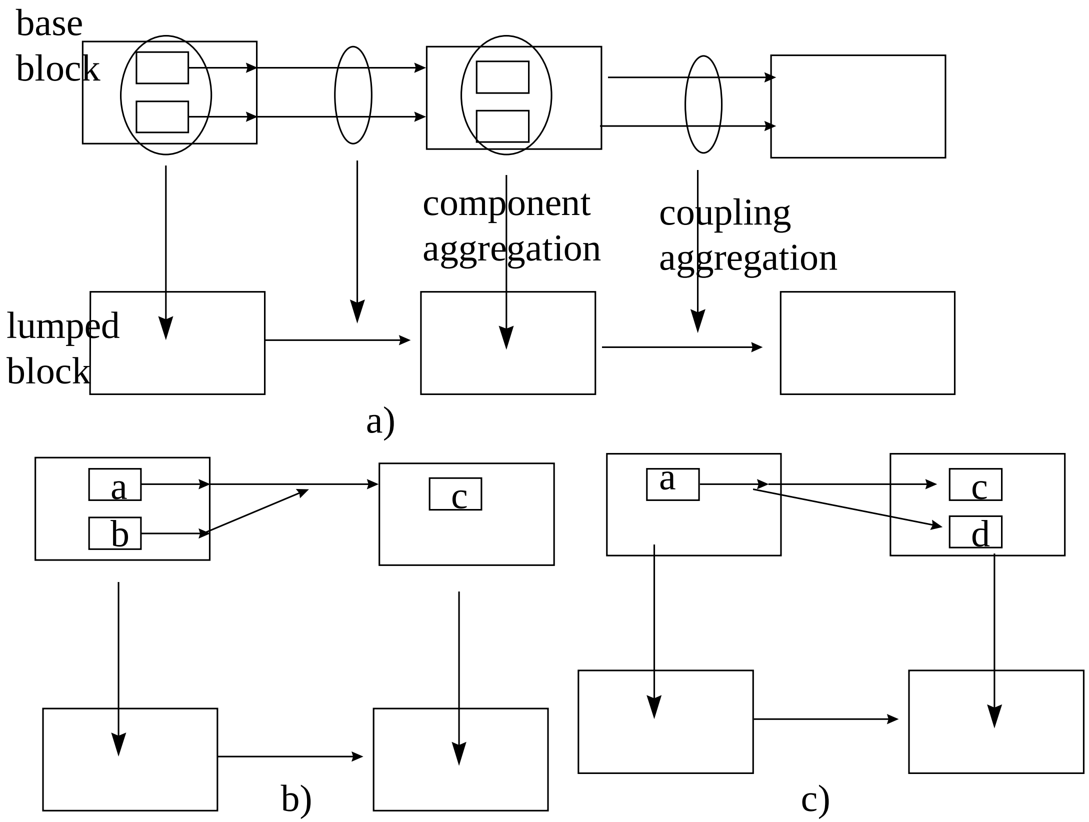


Parameter Morphism: a homomorphism that maps the parameter space of the base model into that of the lumped model



Parameter Morphisms retain valid simplification under changes in parameter values
This supports cross-calibration in multi-level, multi-resolution families

System Theory Generalization of Exact Aggregation Conditions



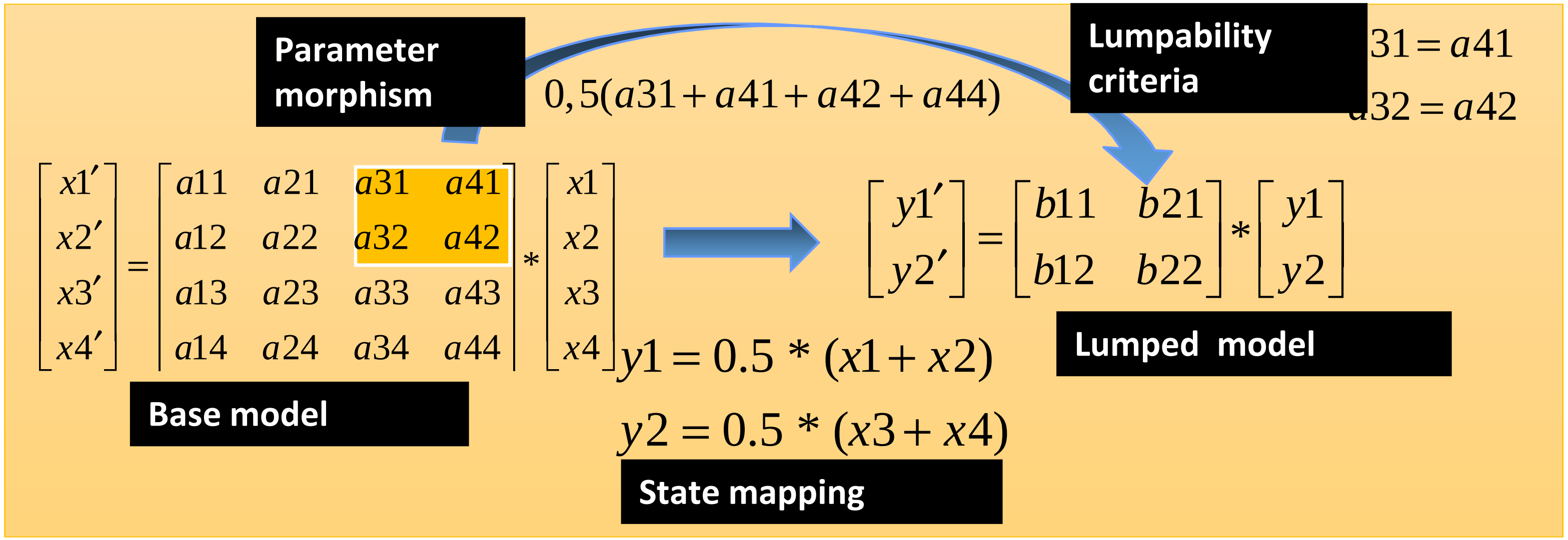
The Aggregation theorem states that not only must there be homogeneity within blocks but also the inter-block element-to-element interactions must satisfy coupling indifference conditions

Theorem: Sufficient conditions for Aggregation

Let there be partition on the components of a base model for wh
homogeneous components, 2) the coupling indifference conditio
and 3) the base model output is computable from block model ce
Then a lumped model exists for which there is an exact homomor
count aggregation.

Example: Lumpability criteria applied to linear discrete time systems

- The base model transition function is expressed as a matrix of coefficients
- The lumped model transition function is of lower order with coefficients derived from aggregation of base coefficients
- The state mapping aggregates base states to lumped states
- Lumpability criteria provide sufficient conditions for preservation of the state mapping over time



Approximate Morphisms handle departures from enabling conditions

- Approximate system morphisms loosen up the strict requirements of exact system morphisms
- Propagation of error that results is characterized and related to the dynamics of the resulting lumped model
- The error propagation can grow or attenuate with time depending on lumped model stability characteristics

- **We can**
  - **analyze a base model and a block partition construction for error departure from exact morphism conditions**
  - **simulate and compare base and lumped model behavior for sensitivity to error propagation**

Example of error propagation analysis: Approximate Lumpability

$$error(t) = \sqrt{(x1 + x2 - y1)^2 + (x3 + x4 - y2)^2}$$

$$\begin{bmatrix} 0 & 0 & g-e & g \\ 0 & 0 & 0 & e \\ 0,5g & 0,5g & 0 & 0 \\ 0,5g & 0,5g & 0 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & g \\ g & 0 \end{bmatrix}$$

Theory predicts that the gain, g determines error propagation characteristics:

- Error decreases over time when g<1
  Otherwise it increases
- The closer to lumpability, the faster the error disappears

g	***e***	**error at time 5**	**error behavior**
0.8	0.001	-0.002	error decreases over time
0.8	0.01	-0.02	decreases
0.8	0.1	-0.2	decreases
0.8	0.0	0.0	constant
1	0.1	0.4	error increases over time
1.2	0.1	7.0	increases explosively

Application to evolving model approximation families

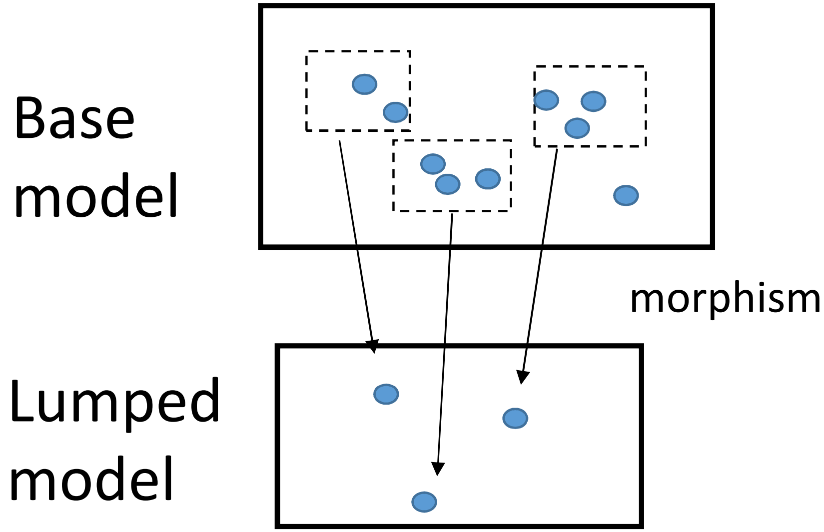
- Approximate model construction methodology supports integrated families of approximate models

- Approximate models are indexed by the experimental frames in which their conditions approximately hold – error propagation conditions in these frames can be estimated

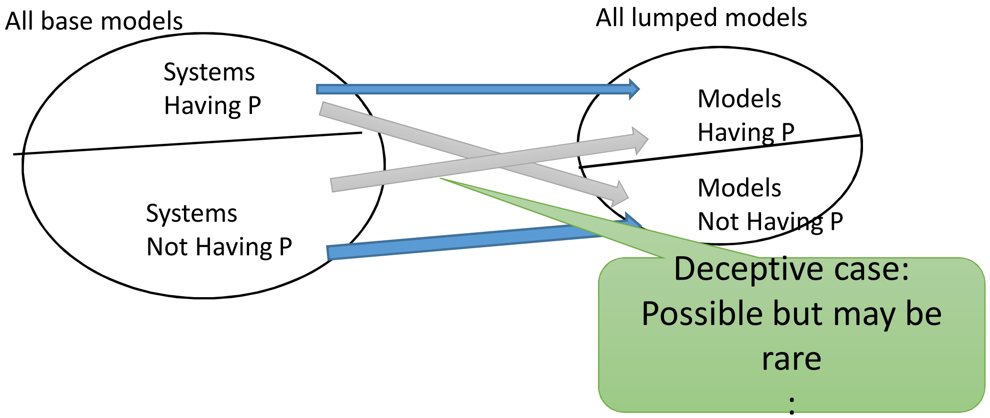
- As field data is ingested for V&V, calibration of any one model propagates information to others from which it is derived and which are further approximations of it, thus maintaining a coherent model family

integrated families of approximation models support 1) estimating trade-offs in accuracy and execution time and 2) choice of approximations meeting analysis needs and time constraints.

Preservation/Predictive Ability (“predictivity”) of models



- Preservation: Does the lumped model preserve a given property of the base model?
- Predictivity: Does a given property of the lumped model imply that the property holds for the base model?
- **Example**: Recurrent (cyclic) vs Absorbing (acyclic) behavior



Lyndon's theorem for automata:
S has positive P implies M has P
M has negative P implies S has P

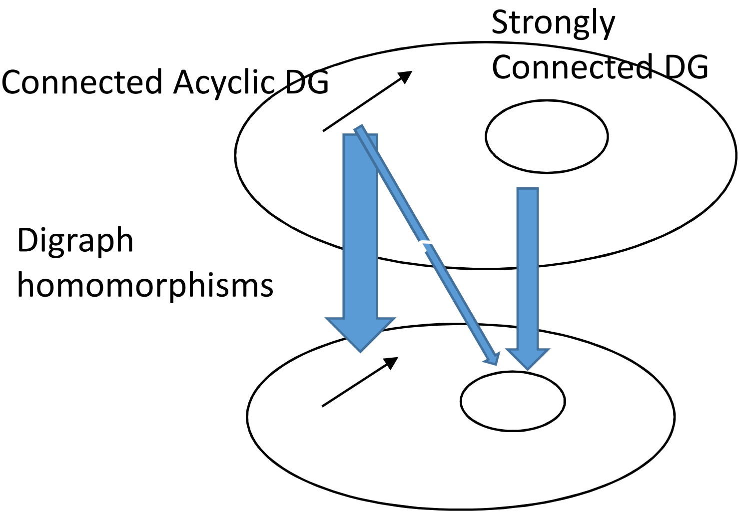
a positive property is one expressible in first order logic without use of negation.

a negative property is one that requires negation to express it.

- Conditions for inheritance of stability properties for continuous systems (Foo)
- Downward preservation of p implies upward preservation of –p
- Properties of interest seem not to be expressible in negative form.,
- Sierocki applied Lyndon's theorem to finite automata.
- Reachability, connectedness, and reversibility and are positive by direct statement.
- Sierocki shows that upward inheritance of positive properties holds for the usual homomorphism of automata.
- Moreover, downward inheritance holds for negative properties.

- Saadawi and Wainer showed that some properties flow upward from safety timed automata models verified in uppaal to real time advance devs models under a strong form of bi-simulation similar to isomorphism.

Preservation/Predictive Ability ("predictivity") of Markov models from analysis of their underlying Directed Graphs(DG)



- Sequences (DAG) can map to DAGs and to Cycles (with low probability)
- Cycles (DCG) can map to **only** DCGs - a cycle either maps to a single state (if it is all in an equivalence class) or to a proper cycle*

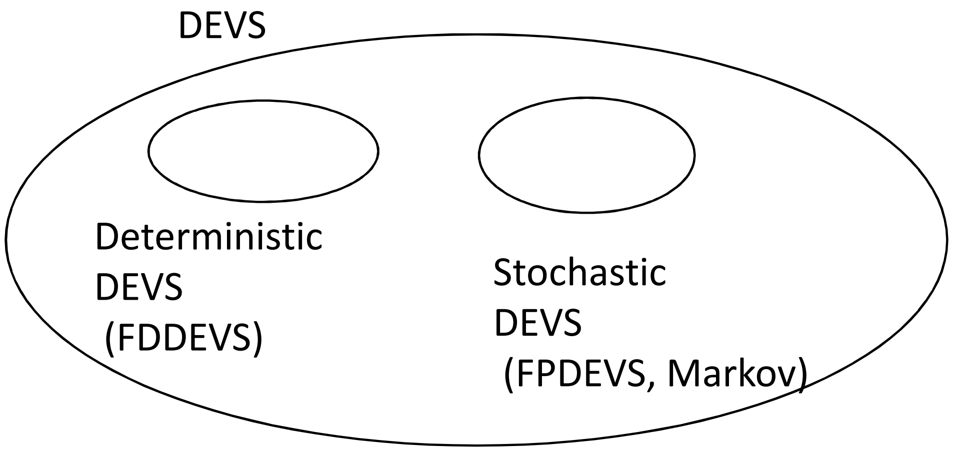
So

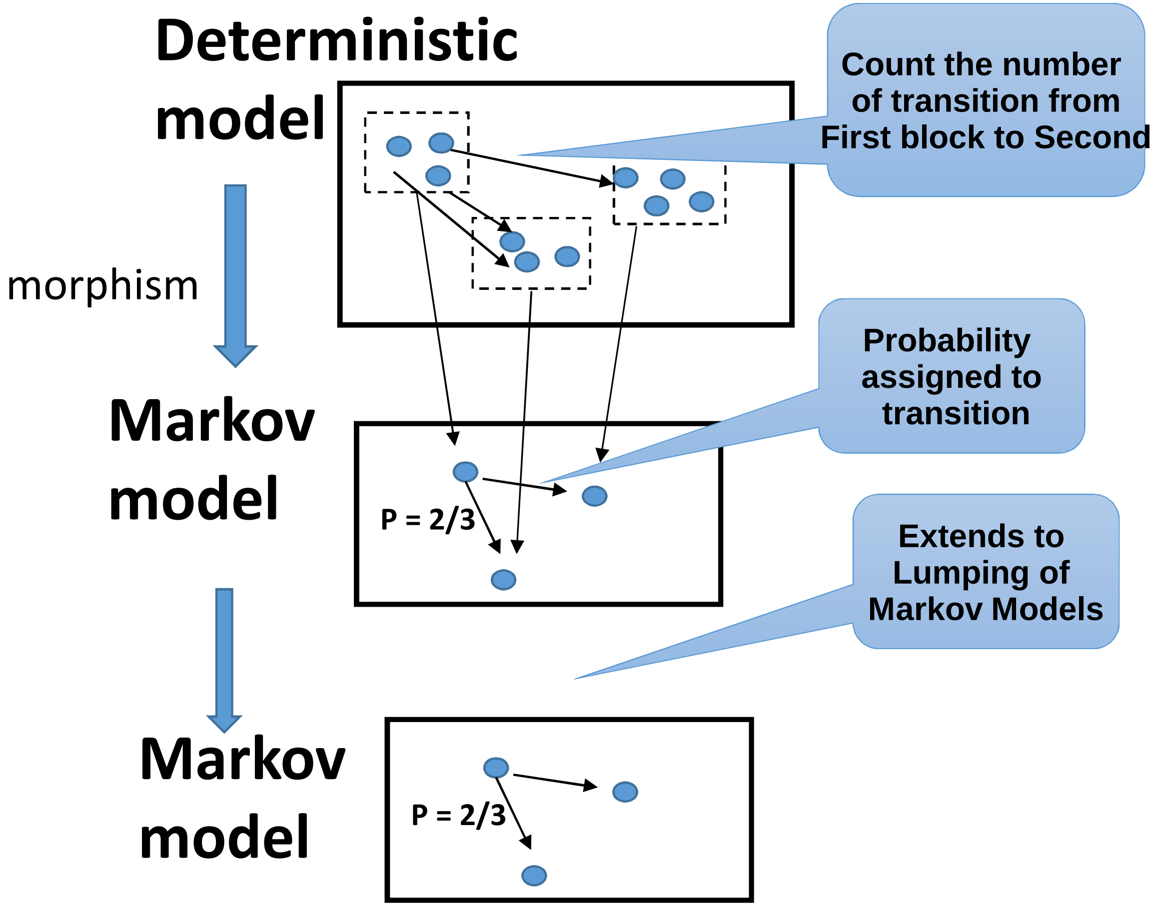
- Lumped Model cycles can only come from Base Model cycles
- Lumped Model sequences come from sequences with high probability
- So (Property Preservation)
- Base Model is recurrent implies Lumped model is recurrent
- Base Model is absorbing implies Lumped model is probably absorbing
- And (Property Predictivity)
- Lumped Model is recurrent implies Base model is probably recurrent
- Lumped Model is absorbing implies Base model is absorbing

* Theorem If C is a directed cycle, then G hom→ C iff G contains only cycles of length divisible by the length of C

Pavol Hell, Huishan Zhou, Xuding Zhu Homomorphisms to oriented cycles. 2003

DEVS makes it easy to cross deterministic /stochastic lines





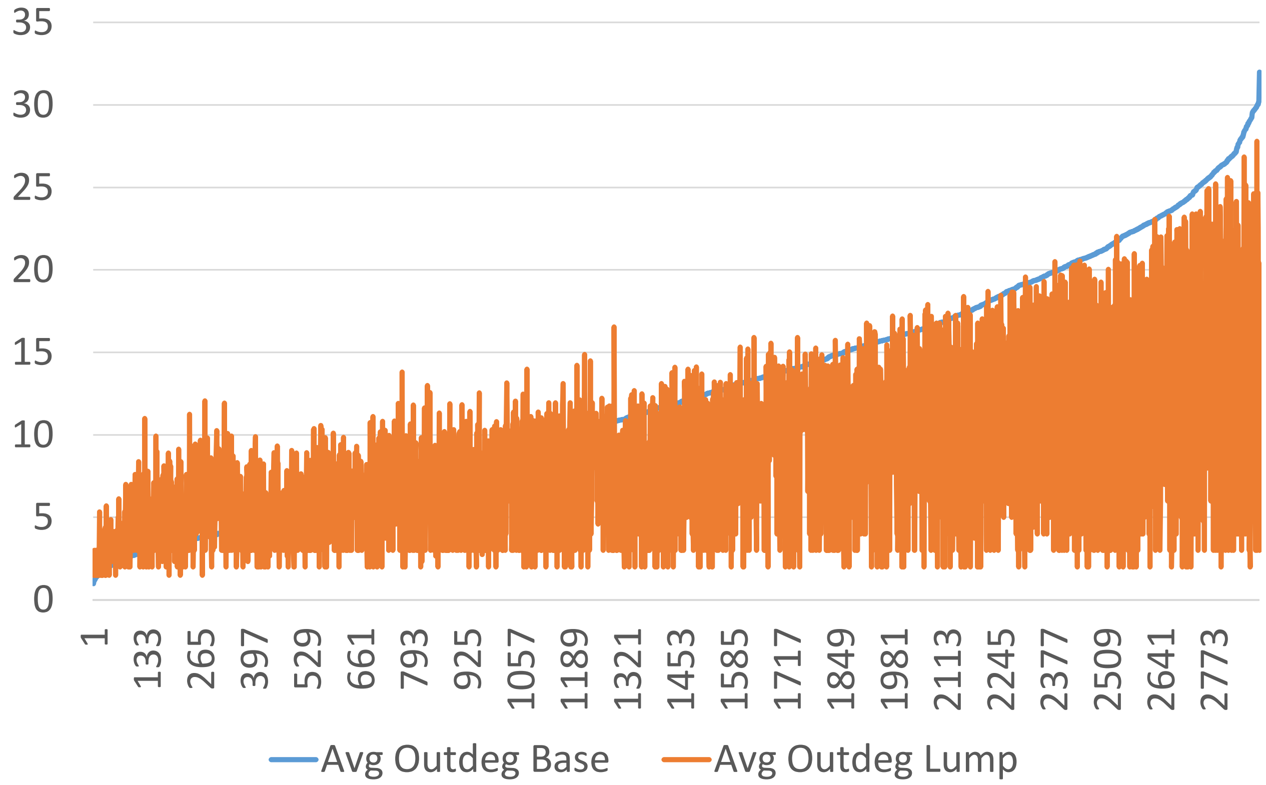
Generated 10,000 pairs of randomized stochastic matrices and state partitions

- The square matrices were sampled from a uniform distribution of sizes, m in the range [4, 34] with partitions sampled conditionally on m with uniform distribution in the range [2,m-1].
- Matrices were generated as sequences of m*m entries sampled with Binomial distribution with probability increased in 10 steps from .1 to 1 each with 1000 trials (with normalization to assure row summation to unity).
- Partitions were generated by partitioning the integer m, selecting one randomly, and randomly permuting the order of the partition numbers
- For each (matrix, partition) pair, the lumped matrix was generated using Equation 1 (Definition 2) so that the original and lumped chains are called the base, lumped model pair.

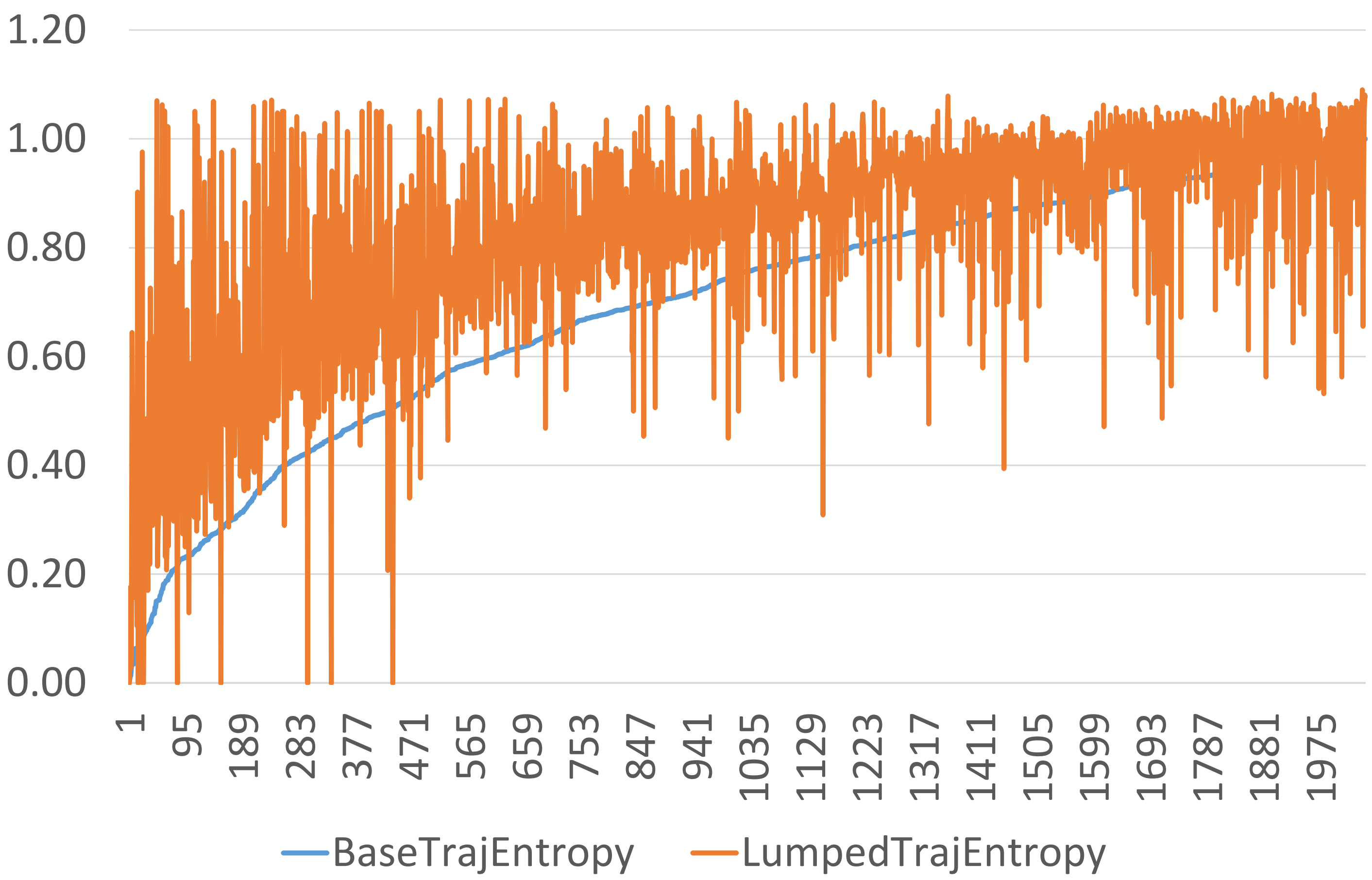
Frequencies of Base/Lumped Cycle Numbers using Cycle Detection in Jama package

Base	Lumped	Number
0	0	38
0	1	147
1	0	28
1	1	9569
1	2	2
2	0	4
2	1	180
2	2	10
3	1	19
3	2	1
4	1	2

Lumping usually reduces the number of transitions: Avg Outdegree of Lumped is usually less than Base



However, Predictive uncertainty is increased by Lumping:
Trajectory Entropy of Lumped usually larger than that of Base



Lumpability example taken from Wikipedia

Prob of transition
Of state 1 to state 2

Sums along rows
= 1

Morphism maps
along row
into their sum

Note
these sums
are equal

$$P = \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} \frac{1}{2} & \frac{3}{8} & \frac{1}{16} & \frac{1}{16} \\ \frac{7}{16} & \frac{7}{16} & 0 & \frac{1}{8} \\ \frac{1}{16} & 0 & \frac{1}{2} & \frac{7}{16} \\ 0 & \frac{1}{16} & \frac{3}{8} & \frac{9}{16} \end{pmatrix} \end{array}$$

Partition maps
States 3 ,4 into
state 2

Partition maps
States 1,3 into
state 1

$$P_t = \begin{array}{c} \begin{array}{cc} 1 & 2 \end{array} \\ \begin{pmatrix} \frac{7}{8} & \frac{1}{8} \\ \frac{1}{16} & \frac{15}{16} \end{pmatrix} \end{array}$$

This morphism is preserved under
Single step transitions

the lumped model has the same
long run behavior as the base

But what about this matrix?
It still is stochastic but does not satisfy lumpability

+ eps

- eps

$$P = \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} \frac{1}{2} & \frac{3}{8} & \frac{1}{16} & \frac{1}{16} \\ \frac{7}{16} & \frac{7}{16} & 0 & \frac{1}{8} \\ \frac{1}{16} & 0 & \frac{1}{2} & \frac{7}{16} \\ 0 & \frac{1}{16} & \frac{3}{8} & \frac{9}{16} \end{pmatrix} \end{array}$$

However it is close
To the original so shouldn't
Its behavior also be close?

+ eps/2

- eps/2

$$P_t = \begin{array}{c} \begin{array}{cc} 1 & 2 \end{array} \\ \begin{pmatrix} \frac{7}{8} & \frac{1}{8} \\ \frac{1}{16} & \frac{15}{16} \end{pmatrix} \end{array}$$

Lumpability metric: LumpSTD measures how varied the partial sums are – the more varied the less lumpable

$$
\begin{array}{cc}
 & \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\
P = & \begin{pmatrix} \frac{1}{2} & \frac{3}{8} & \frac{1}{16} & \frac{1}{16} \\ \frac{7}{16} & \frac{7}{16} & 0 & \frac{1}{8} \\ \frac{1}{16} & 0 & \frac{1}{2} & \frac{7}{16} \\ 0 & \frac{1}{16} & \frac{3}{8} & \frac{9}{16} \end{pmatrix}
\end{array}
$$

$$
\begin{array}{cc}
 & \begin{array}{cc} 1 & 2 \end{array} \\
P_t = & \begin{pmatrix} \frac{7}{8} & \frac{1}{8} \\ \frac{1}{16} & \frac{15}{16} \end{pmatrix}
\end{array}
$$

Consider the sums as
samples of a rv
Compute the sample mean and std
The mapped value = sample mean
LumpSTD be the std.

Jensen-Shannon Metric For Probability Distributions

The Jensen-Shannon divergence, defined for two distributions
and Q by

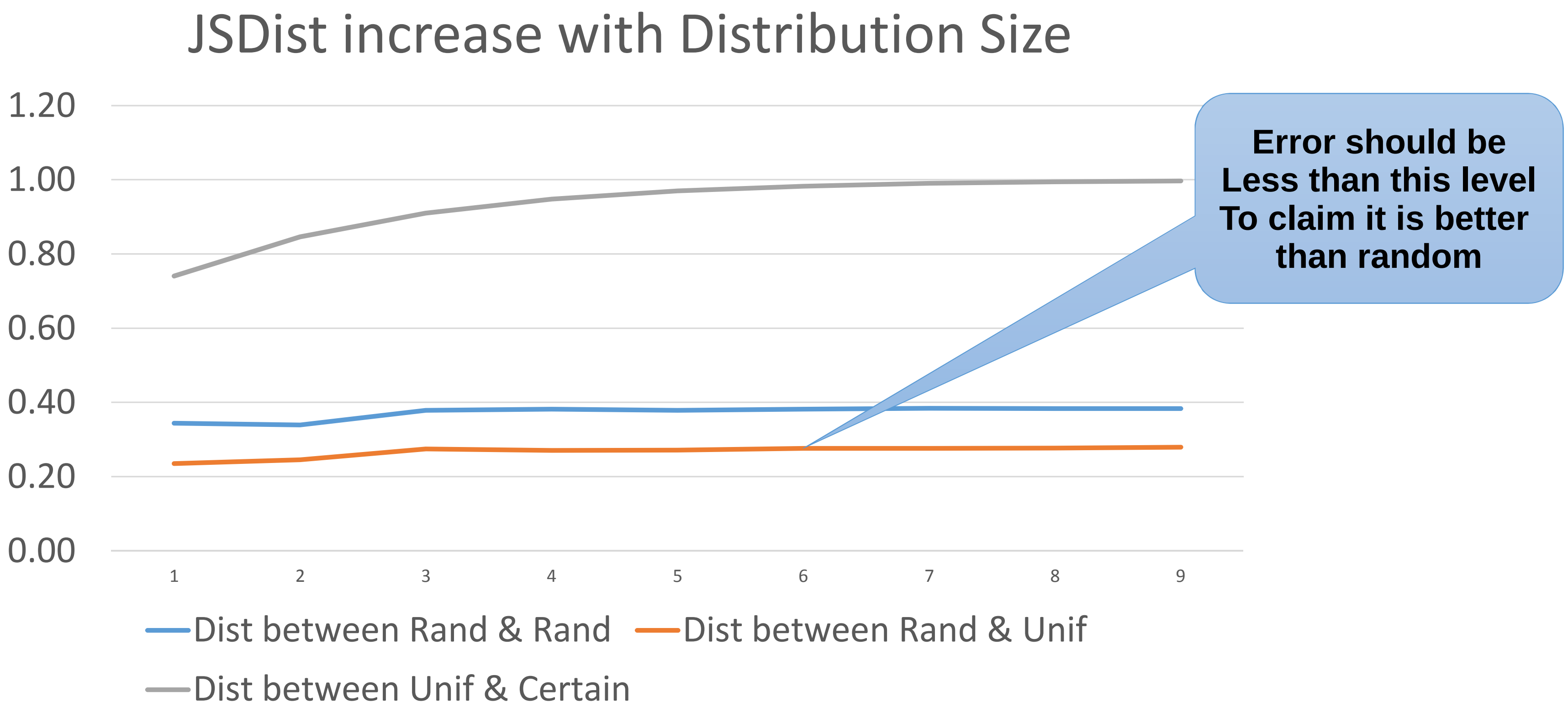
$$JSD(P,Q) = \frac{1}{2}D(P\|M) + \frac{1}{2}D(Q\|M)$$

where $M = \frac{1}{2}(P+Q)$ and $D(A\|B)$ is the Kullback-Leibler

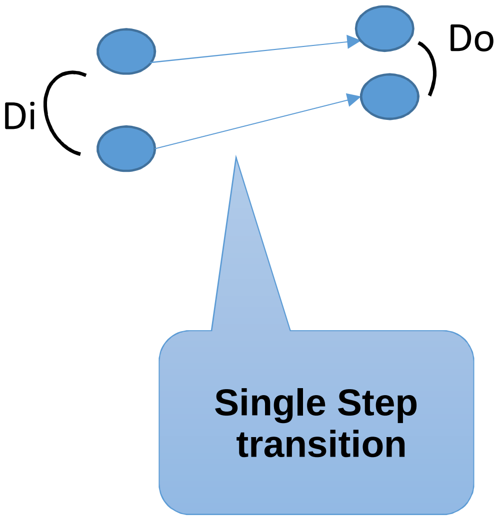
JSDist = square root (JSD) is a distance metric

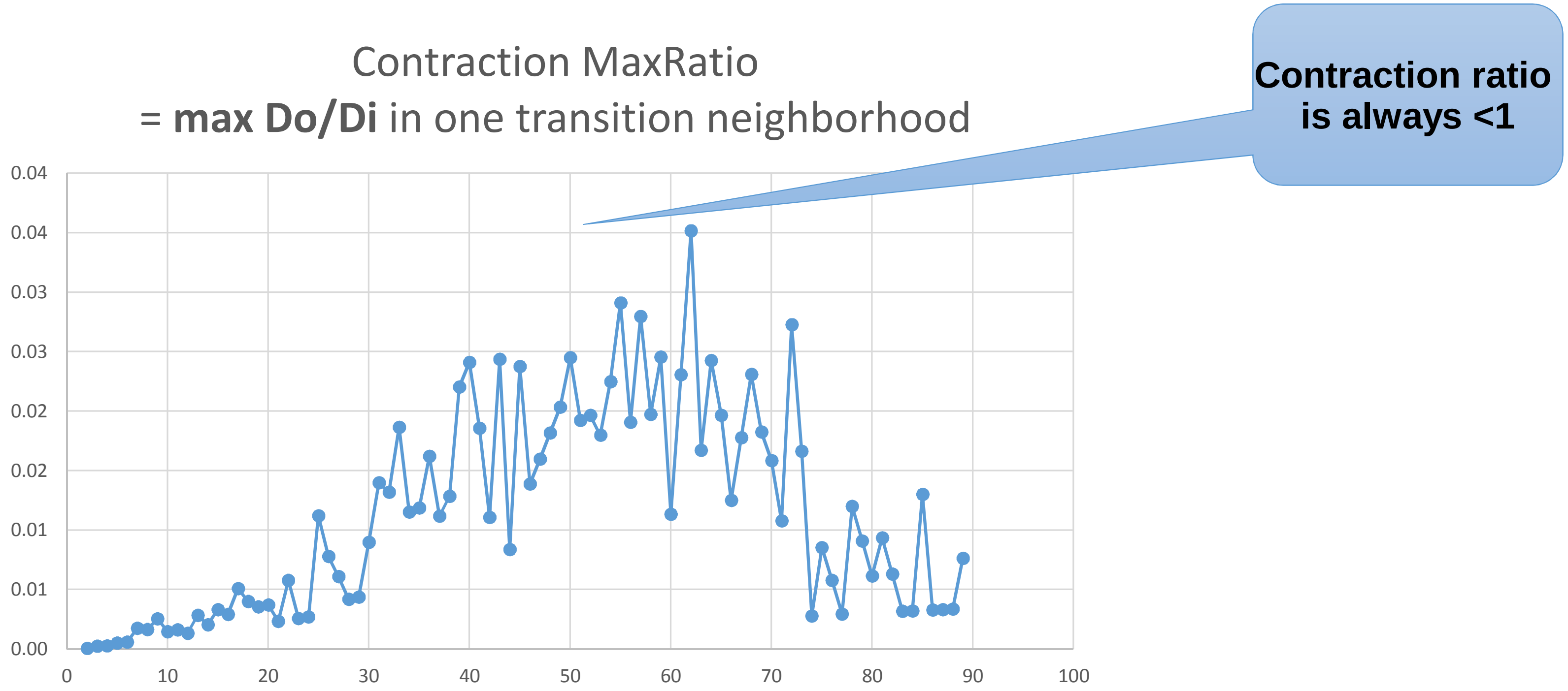
Approximation Error =
JSDist (Lumped Equilibrium Distribution,
Mapped (Base Equilibrium Distribution))

Background values of JSDist metric

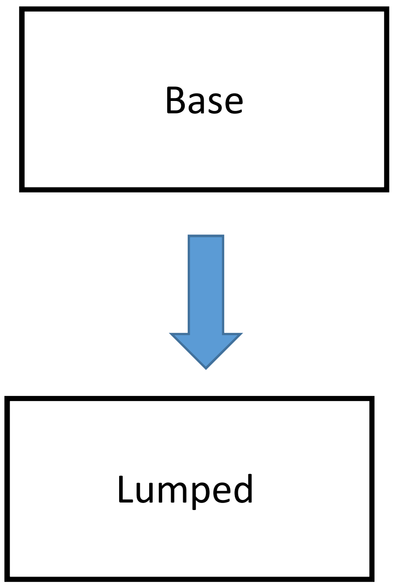


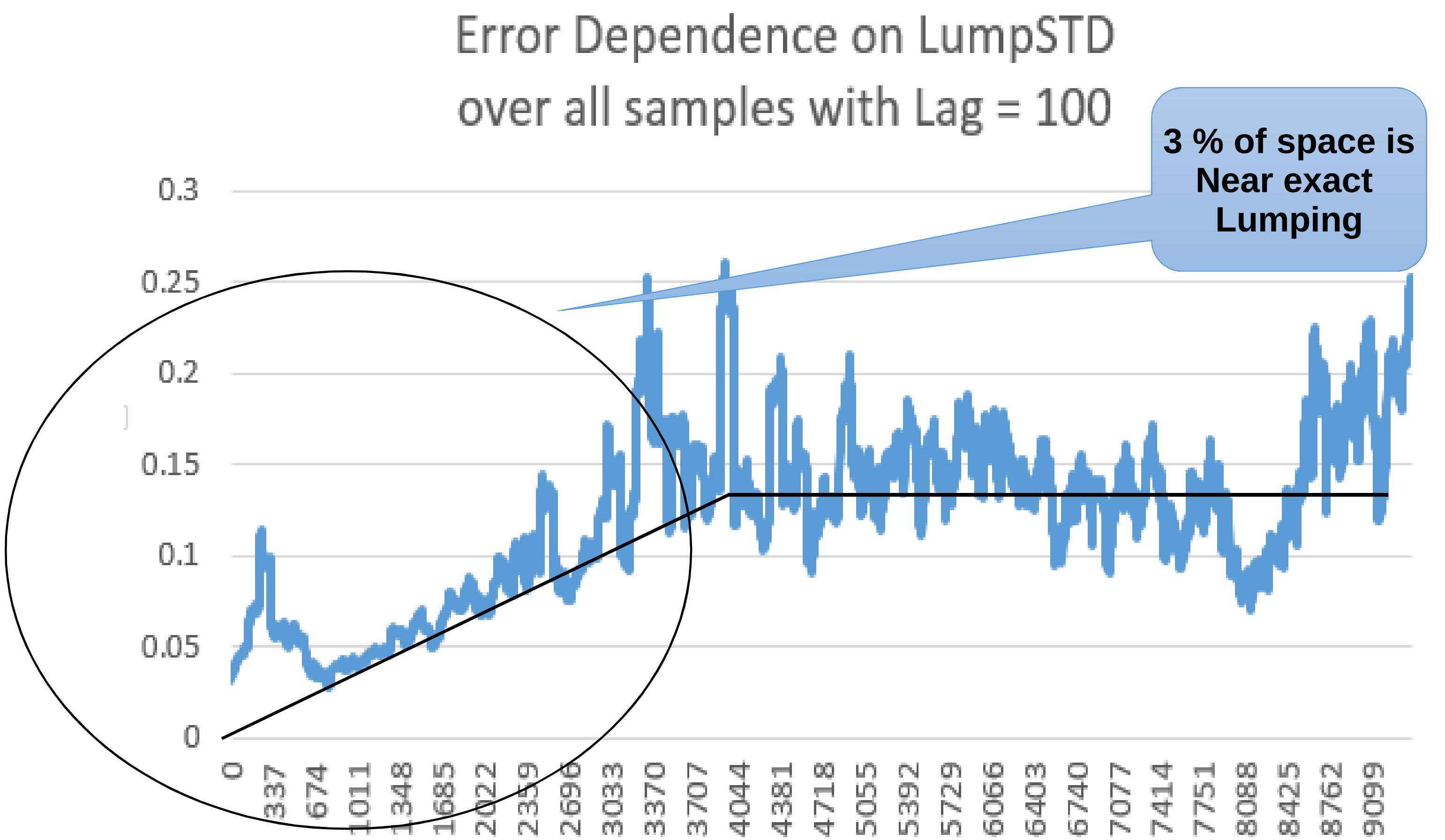
Error propagation is self-damping: general theory says Contraction mapping implies error decreases





Approximate Morphisms: What's the probability of finding a reasonably good approximate lumpable partition when sampling at random?





Conclusion

- Properties of interest may not be preserved in the abstraction process
- Moreover lumped model properties may be deceptive – they may not carry over to the base model
- Measures of model quality may not behave as expected under aggregation
- Exact morphisms are very rare
- But approximate morphisms may be much more common and discoverable by modelers – humans and computers