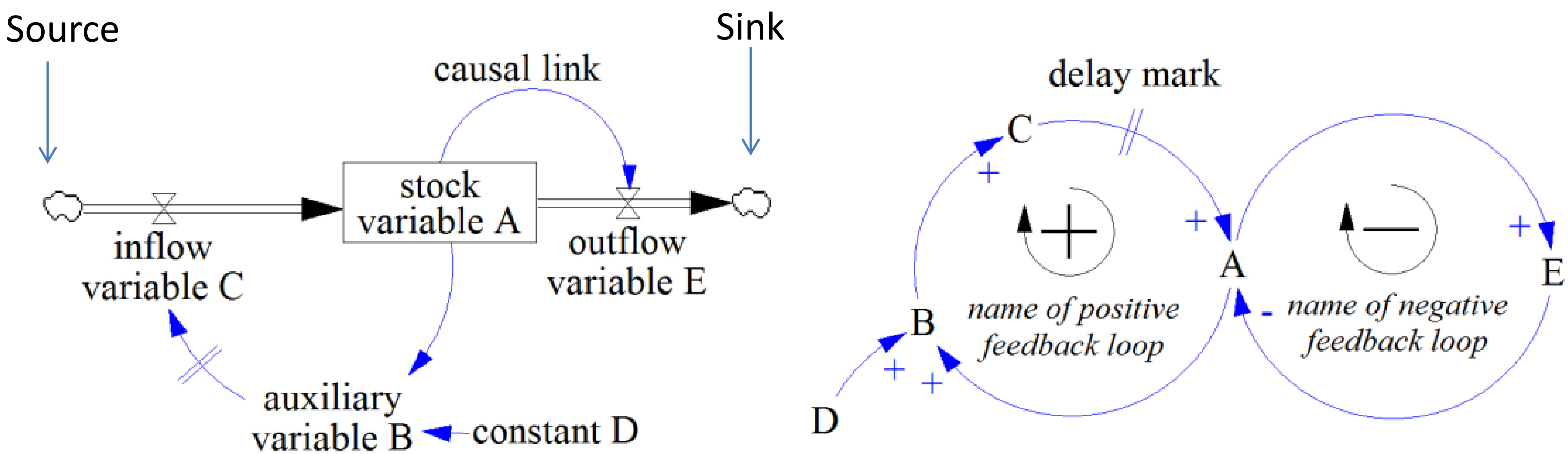
Simulation and Analysis on Steroids with Python

Erik Pruyt

Overview

1. Traditional System Dynamics Model. & Simulation
2. EMA Workbench & AS: Simulation & analysis with Python scripts and ipython / jupyter notebooks
3. PySD: Translating Vensim models to Python + Calibration, Simulation & Analysis in Python
4. From Aggregated to Disaggregated and Hybrid Modelling & Simulation
   (3) Database + 1 model for many regions (wo interaction)
   (4) MSc thesis of Philipp Schwarz
   (5) Hierarchical geo-spat. SD-ABM-DES M&S in AnySim

Traditional System Dynamics Modelling & Simulation

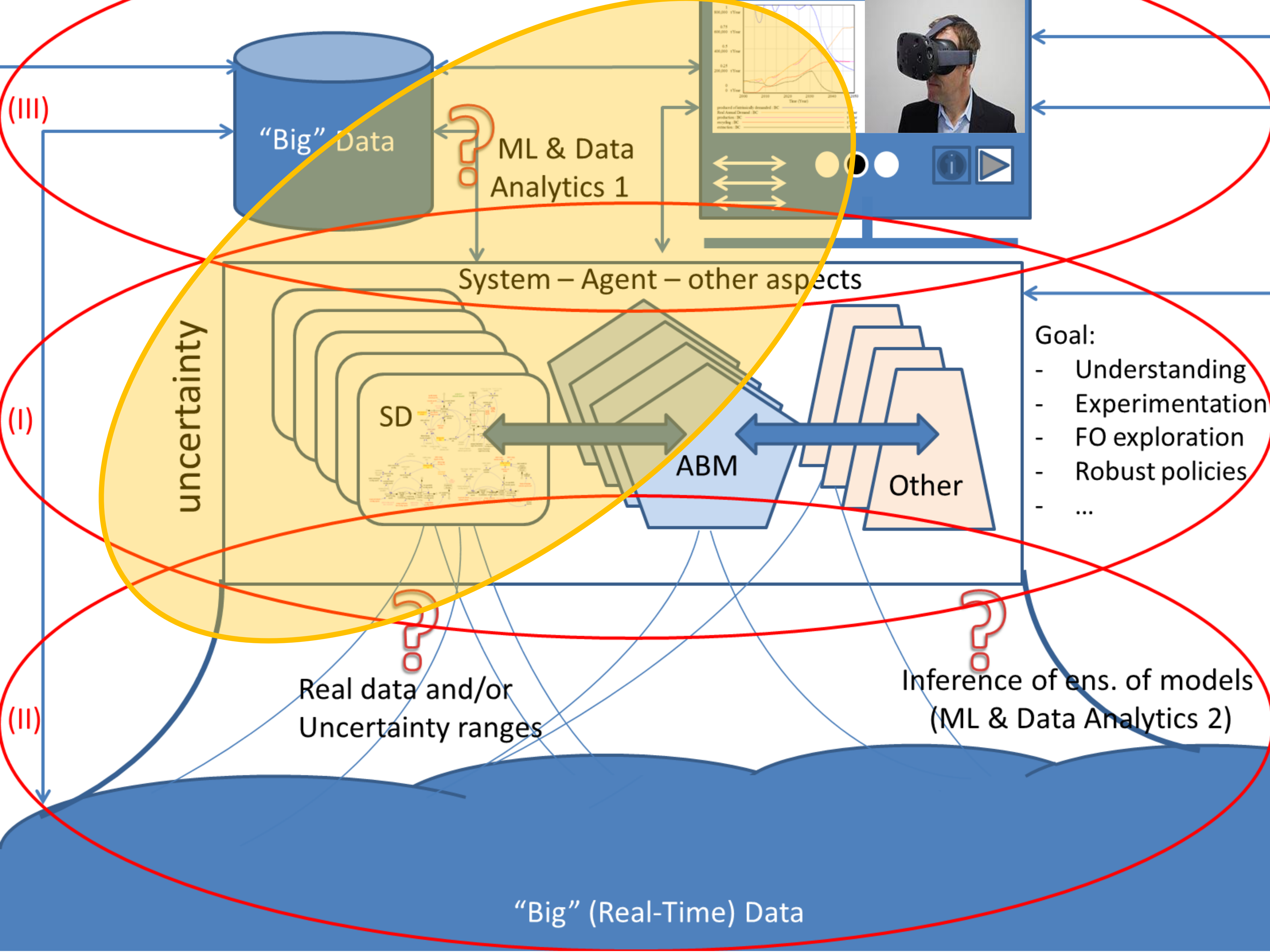


- Causal Loop Diagrams -> causal effects and feedback loops
- Stock Flow Diagrams -> ``Simulation Models´´:

  Stocks, flows, delays, auxiliaries, parameters, (sources and sinks)
- Hybrid Diagrams -> Causal Loop Diagrams + Stocks (&Flows)

Overview II: Enhancing SD with Python

- Pre 2009: “traditional” System Dynamics modelling
- “Trying” to do uncertainty & robustness analysis
- 2009: Dynamic complexity x “Deep Uncertainty”, first w Caner Hamarat , later w Jan Kwakkel et al.
- Mexican Flu: model in 30’ + 3 weeks of exploration
- Post ” ”: case-based development -> **EMA wrkbnch**
- 2015: Workshop setting? => “**Adaptive Sampling**”
- 2015: **pySD** (James Houghton @ MIT)
- 2016: **python+** (Philipp Schwarz, Bas Keijser, WLA)
- 2016: **AnySim** (Reza Hesan)



(III)
"Big" Data
ML & Data
Analytics 1
System – Agent – other aspects
uncertainty
SD
ABM
Other
Goal:
- Understanding
- Experimentation
- FO exploration
- Robust policies
- …
(I)
Real data and/or
Uncertainty ranges
Inference of ens. of models
(ML & Data Analytics 2)
(II)
"Big" (Real-Time) Data

1) EMA Workbench, AS2, etc: Simulation & Analysis with Python & jupyter notebooks

- Exploratory Modelling and Analysis
  - Why? What? How?
  - Examples
    - Example 1 - Flu: ExampleFluWithPoliciesV.ipynb & PrimFlu.ipynb
    - Example 2 - Ebola: EbolaV26Models123456wPOLSprimmedV03_overtimeD291UncRed
- Adaptive Sampling (AS2)
  - Why? What? How?
  - Examples
    - Energy/Climate to State Instability
    - BSSv02b_Burnout01short_v01.ipynb

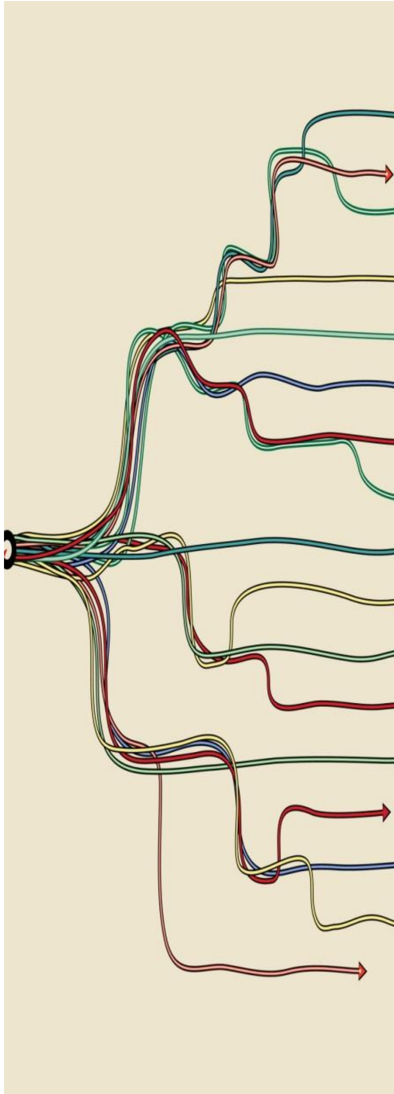
Why?

Deep uncertainty: Uncertainty & Ambiguity

- Decision makers and stakeholders do not know or cannot agree on the outcomes of interest, the system under study, or future developments
- How to let planning and decision making proceed despite the presence of different models, different beliefs about the future, and disagreement on which outcomes of interest should be included?

⇒ Not just sampling across input parameter ranges: inputs (lack/conflict of data/info), perspectives (different models), evaluation of desirable, methods,…

⇒ Sets of plausible models of the system, of outcomes of interest without a priori weighting, and of scenarios



Approaches for Dealing with Uncertainty, Ambiguity and Surprises in modelling

- Explorative modelling: embrace uncertainty, model un/knowns and multiple perspectives, what-if explorations / test policy robustness
  - => Inclusion of different models, relations, inputs,…
- Consolidative / consensual modelling: reduce uncertainty as much as possible, model "known"/agreed upon, and test sensitivity
- Steps still +/- the same, but everything changes

What? Exploratory Modelling & Analysis

Model-based methodology for systematically exploring deep uncertainty & testing policy robustness

1. Identification of 'certainties' and 'uncertainties' **&** construction of 'plausible' SD model**s**

2a. Open exploration

1. Model-based generation of many plausible scenarios
2. Analysis of ensemble of plausible scenarios using all sorts of algorithms (clustering, PRIM, …)
3. Identification of interesting types of scenarios + origins

2b. Direct searches

3. Policy design and testing across all plausible scenarios

- Need for fast and manageable models… => SD!!!

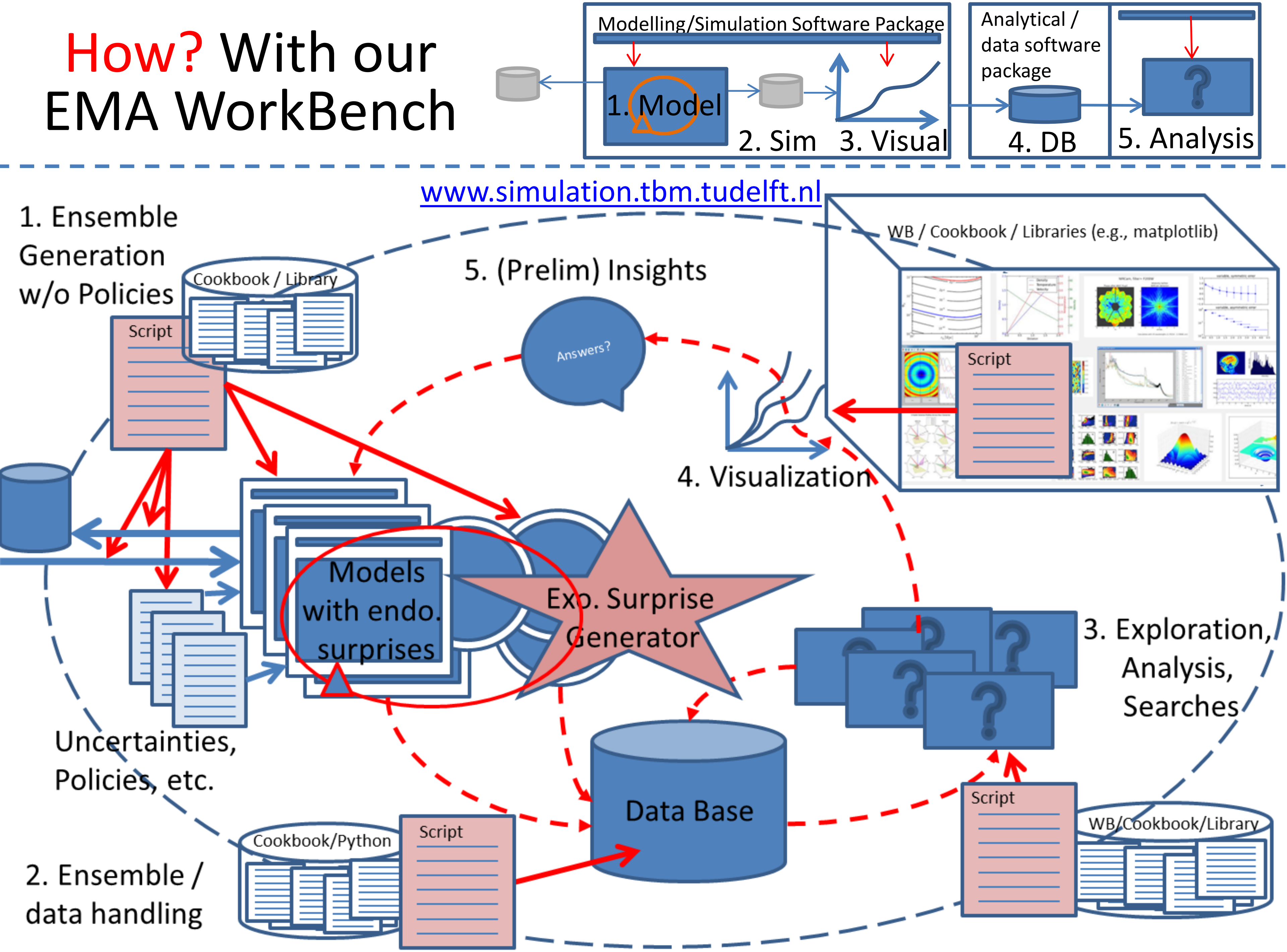
Open exploration

- Design of experiments
  - Factorial methods
  - Monte Carlo sampling
  - Latin Hypercube sampling
  - Behaviour Space sampling
- Used for
  - Identification of bandwidth outcomes
  - Identification of types of behavior
- Subsequent analyses
  - Scenario discovery
  - (Policy analysis + testing)

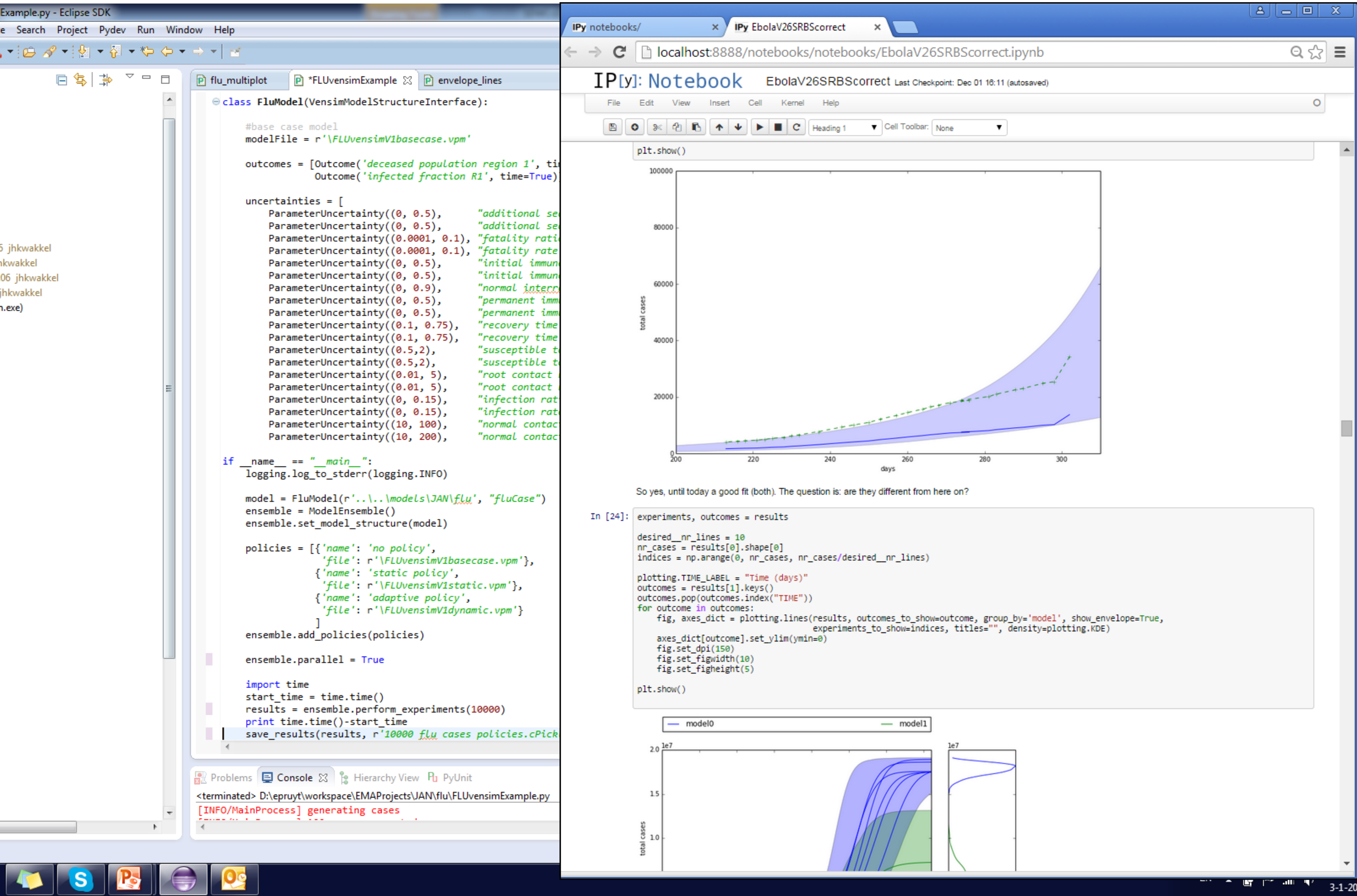
Directed search

- Optimization for search
  - Multi-objective optimization
  - Robust optimization
- Used for
  - Worst case discovery
  - Identification of boundaries where behavior switches
  - Policy design
- Subsequent analyses
  - Trade-offs
  - Tipping points

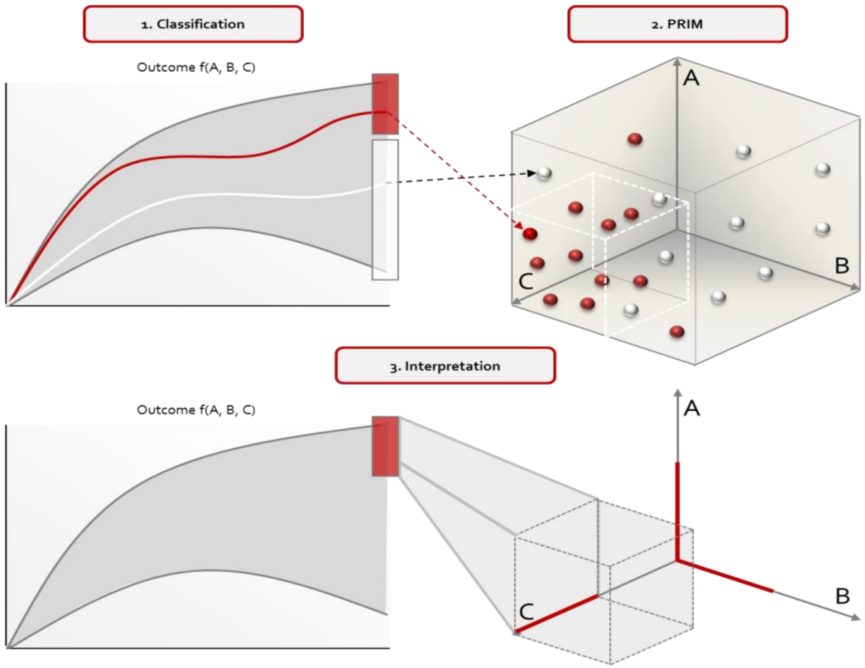
How? With our EMA WorkBench

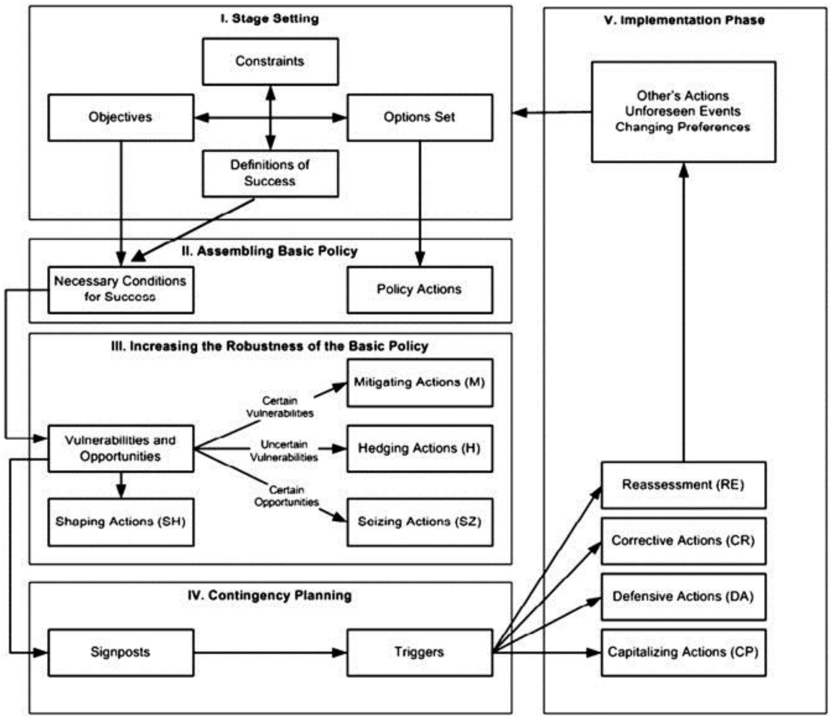


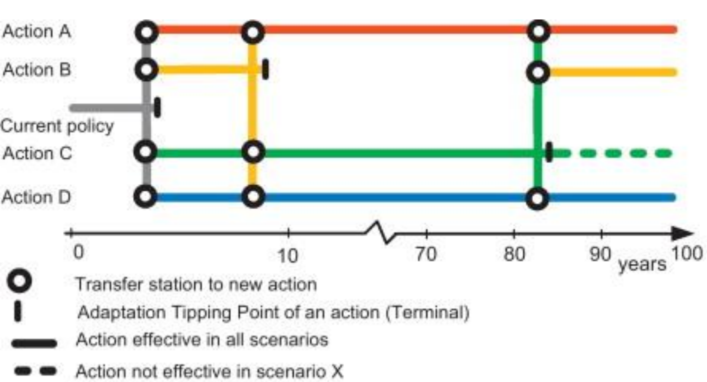
EMA WB, Python, Jupyter Notebooks



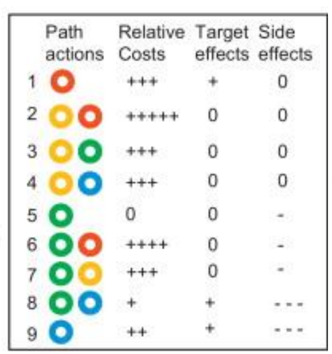
New Methods, Techniques, Algorithms



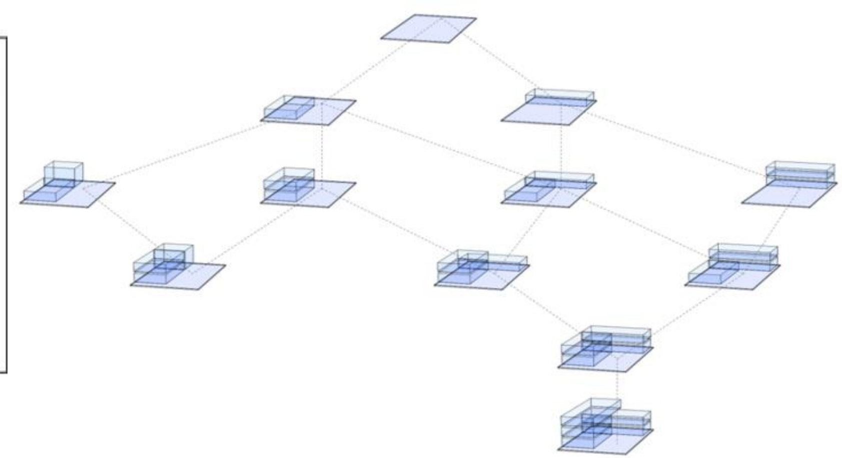




Adaptation Pathways Map



Scorecard pathways

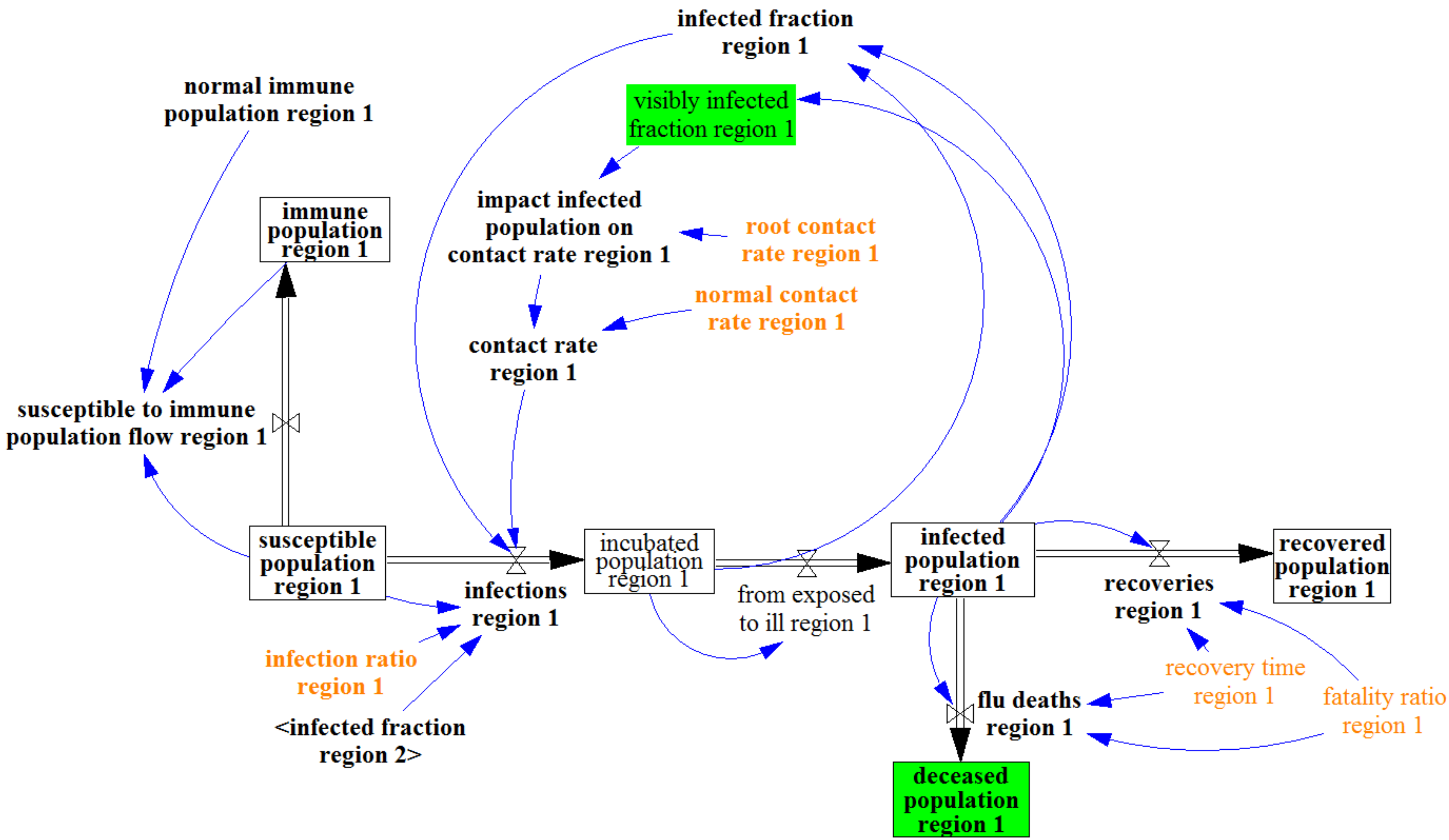


Example 1: 2009 A(H1N1)v

- April 2009: imminent epidemic/pandemic of new flu strand
- **Unknowns!**

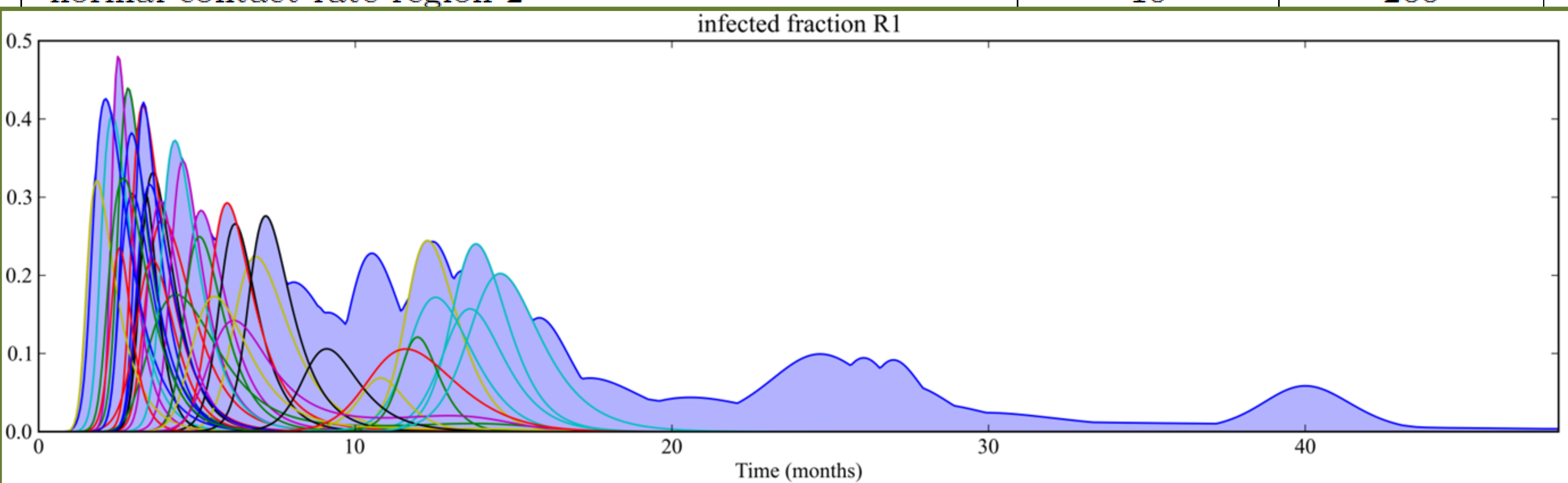
Date	24 April	30 April	08 May	20 May	12 June	20 July	21 August
Infectivity	unknown	unknown	unknown	unknown	unknown	unknown	unknown
Ro	unknown	unknown	1–2; prob. 1.4–1.9	1–2; prob. 1.4–1.6	–	–	[R up to 2]
Immunity	unknown	unknown	indications (elderly)	idem	idem	idem	idem
Virulence	unknown	unknown	unknown	unknown	unknown	mild and self-limiting	idem
Incubation period	unknown	unknown	long tail? (up to 8d)	–	median 3-4d range 1-7d	idem	idem
CFR (Mexico)	17%?	–	4%?	2%?	0.4–1.8%?	–	–
CFR (USA)	unknown	unknown	0.1%?	0.1%?	0.2%?	0.4%?	–
CFR (UK)	unknown	unknown	unknown	unknown	unknown	0.3%(–1%)?	0.1–0.2%? (0.35% ¬ ex.)
Age distribution	unknown	unknown	older people less affected?	–	skewed tow. younger	idem	idem
Antiviral suscep.	unknown	possible	indications	–	–	–	–
% asymptomatic	unknown	unknown	unknown	unknown	unknown	indications	33–50% (ass.)
Future severity?	unknown	unknown	unknown	unknown	unknown	unknown	unknown
Respective sources	(ECDC 2009g)	(ECDC 2009f)	(ECDC 2009b)	(ECDC 2009c)	(ECDC 2009a)	(ECDC 2009d)	(ECDC 2009e)

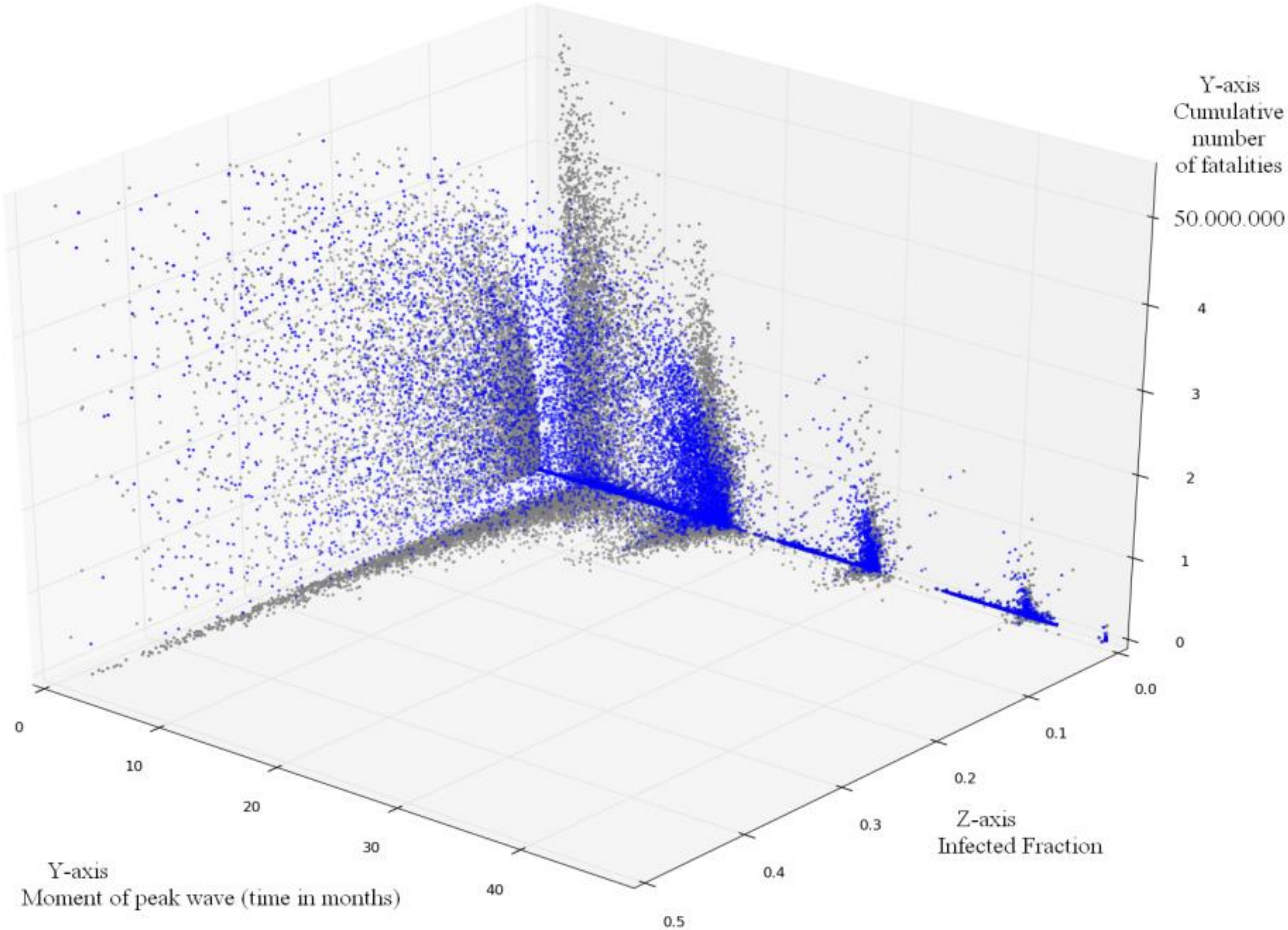
Pruyt & Hamarat 2010



Pruyt & Hamarat 2010

Parameter	Lower Limit	Upper Limit
additional seasonal immune population fraction region 1	0.0	0.5
additional seasonal immune population fraction region 2	0.0	0.5
fatality ratio region 1	0.0001	0.1
fatality ratio region 2	0.0001	0.1
initial immune fraction of the population of region 1	0.0	0.5
initial immune fraction of the population of region 2	0.0	0.5
normal interregional contact rate	0.0	0.9
permanent immune population fraction region 1	0.0	0.5
permanent immune population fraction region 2	0.0	0.5
recovery time region 1	0.2	0.8
recovery time region 2	0.2	0.8
root contact rate region 1	1.0	10.0
root contact rate region 2	1.0	10.0
infection ratio region 1	0.0	0.15
infection ratio region 2	0.0	0.15
normal contact rate region 1	10	100
normal contact rate region 2	10	200

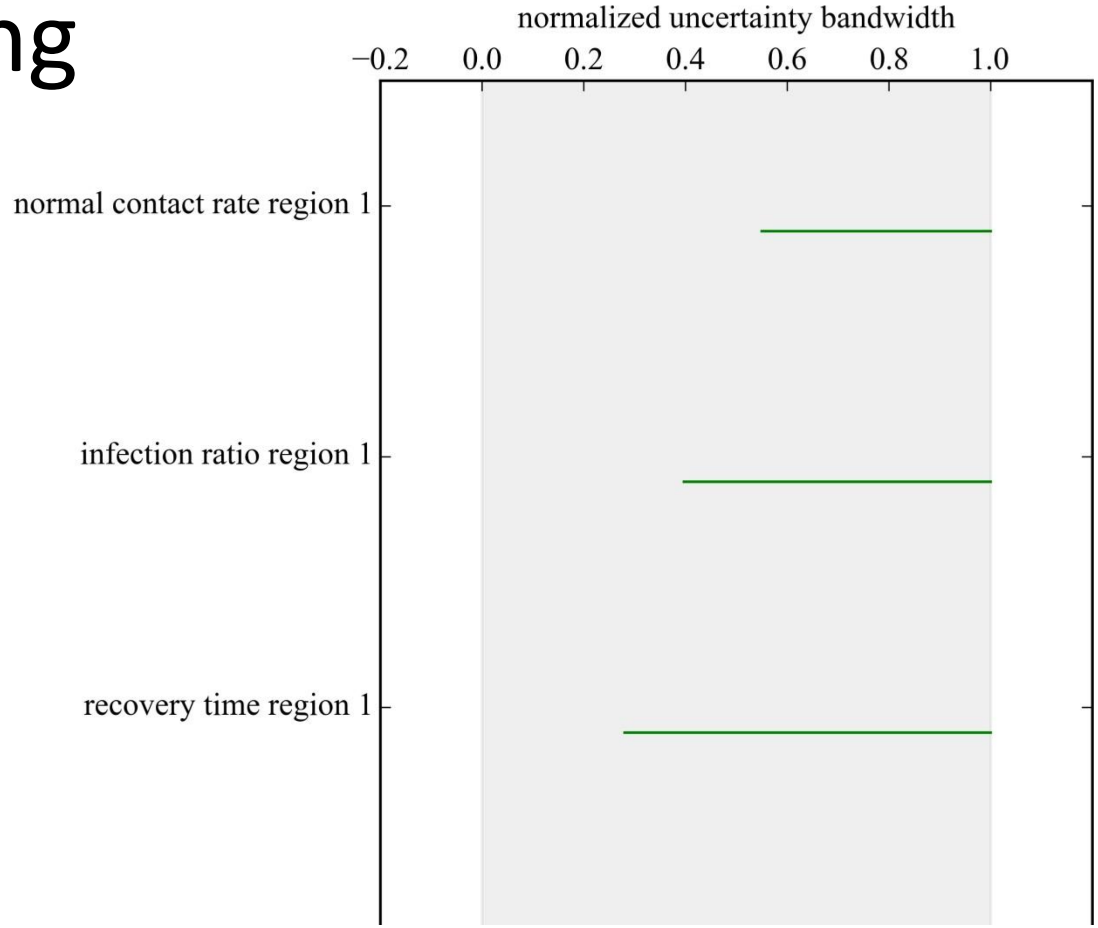




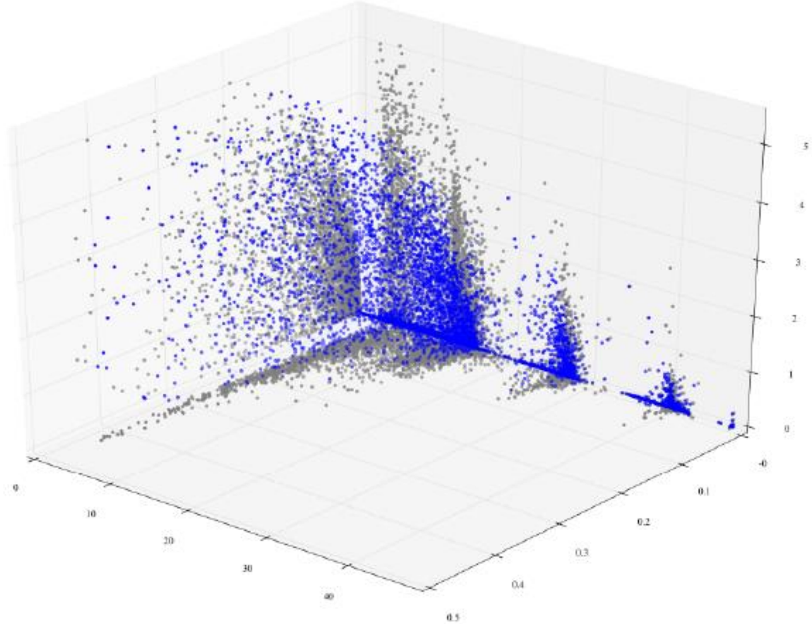
Pruyt & Hamarat 2010

Machine Learning Algorithms

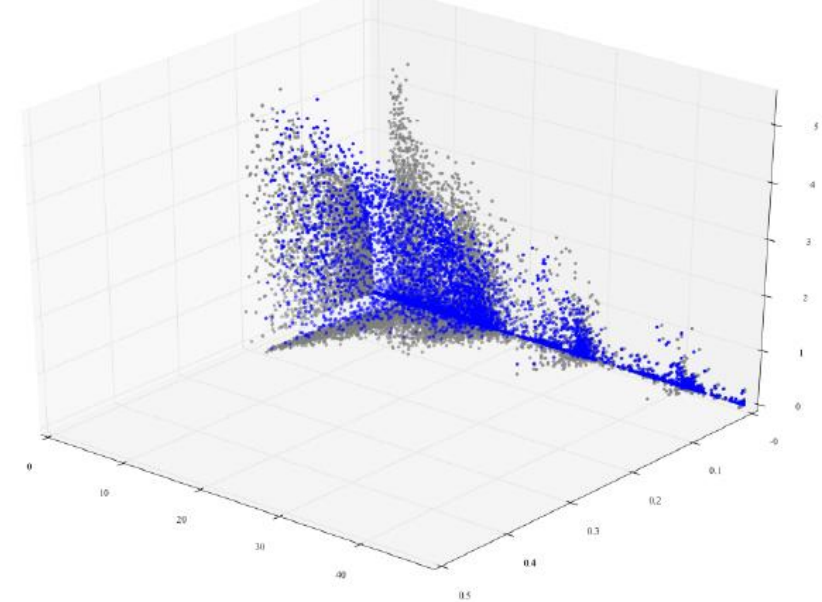
- Combined causes of ° of undes. runs
- Not just parametric
- Dynamics



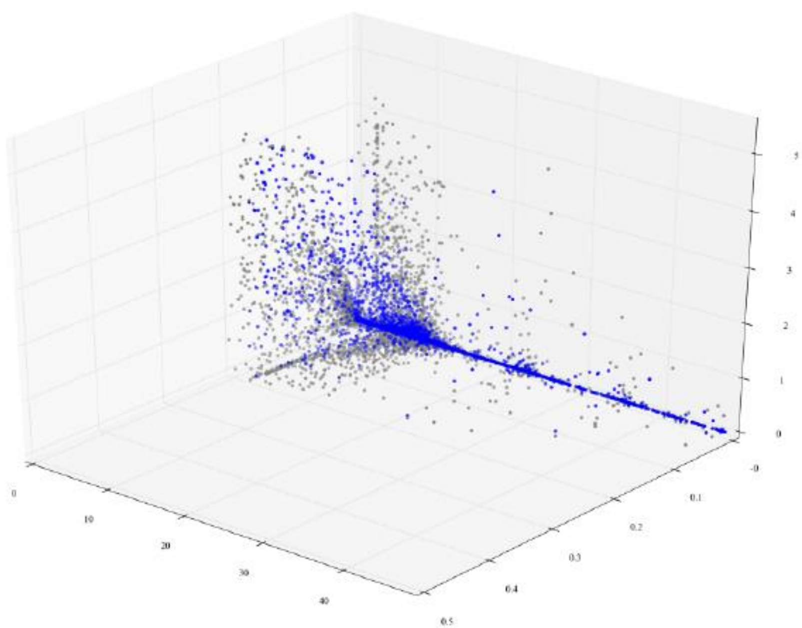
PRIM box bouding uncertainties	box 1: min:	max:	rest box min:	max:
normal contact rate region 1	**59.490**	99.986	10.003	99.986
infection ratio region 1	**0.060**	0.150	0.000	0.150
recovery time region 1	**0.282**	0.750	0.100	0.750
additional seasonal immune pop fraction R1	0.023	0.470	0.000	0.500
fatality ratio region 1	0.010	0.100	0.000	0.100
infection rate region 2	0.014	0.150	0.000	0.150
root contact rate region 1	0.012	4.693	0.014	4.998
permanent immune population fraction R1	0.000	0.478	0.000	0.500



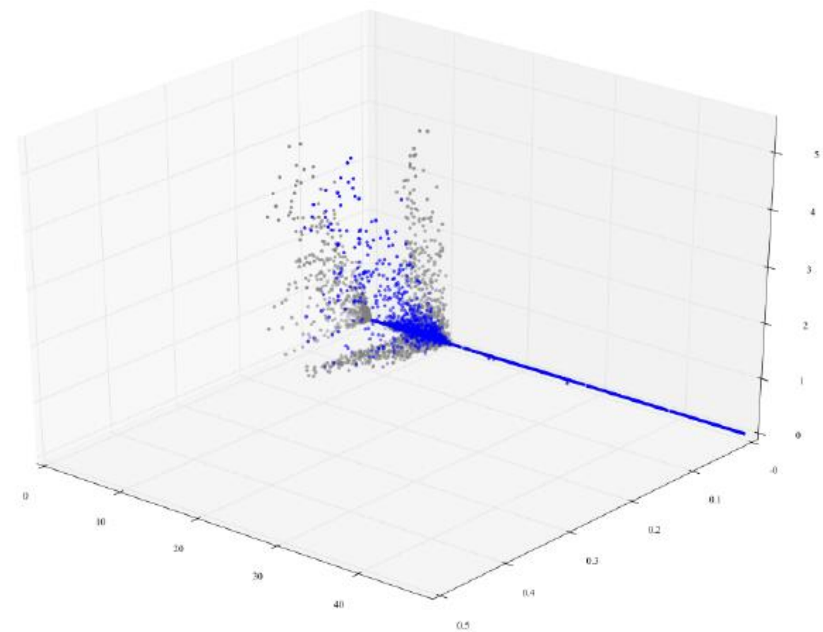
(a) No Policy



(b) Basic Policy



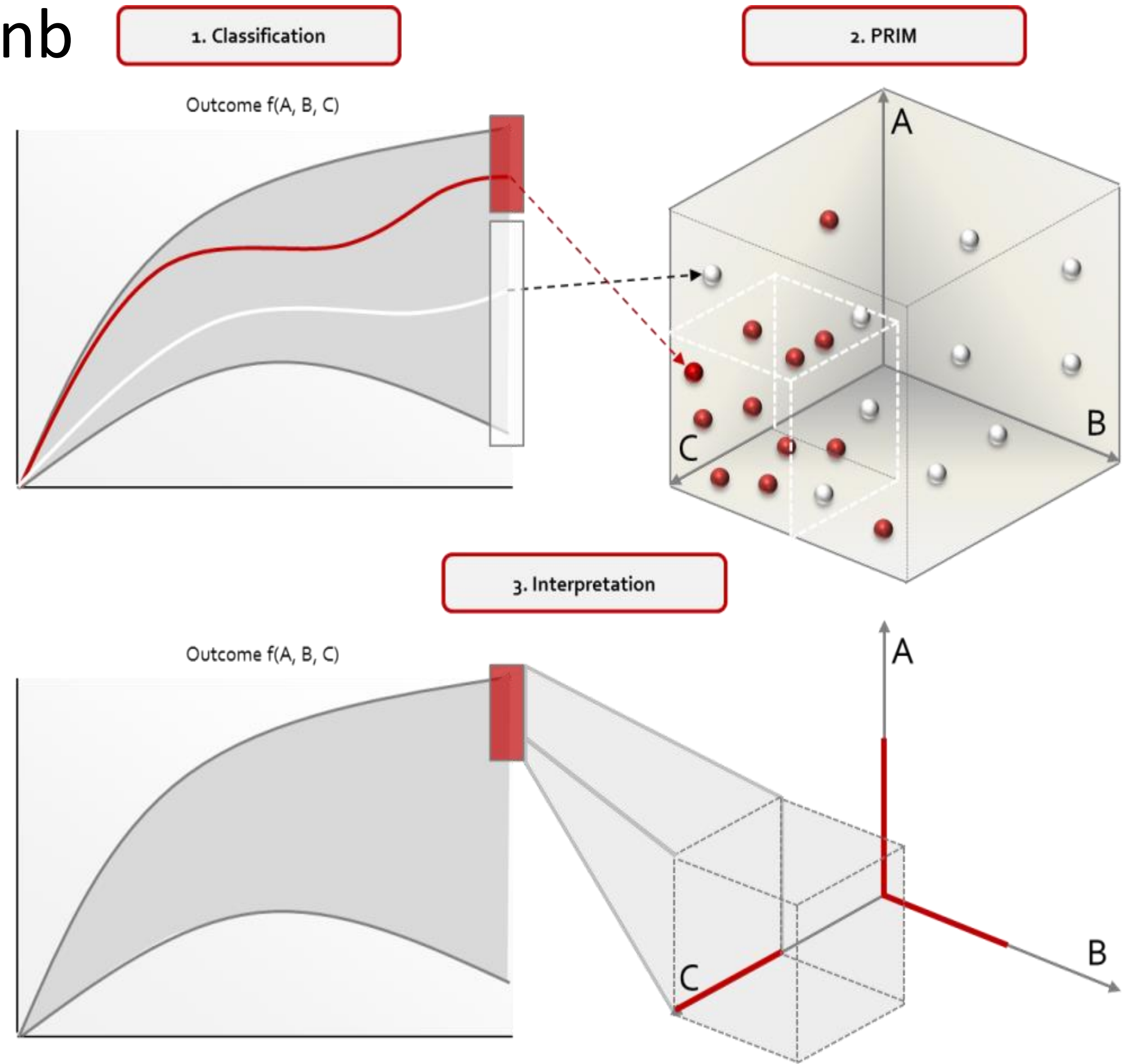
(c) Adaptive Policy



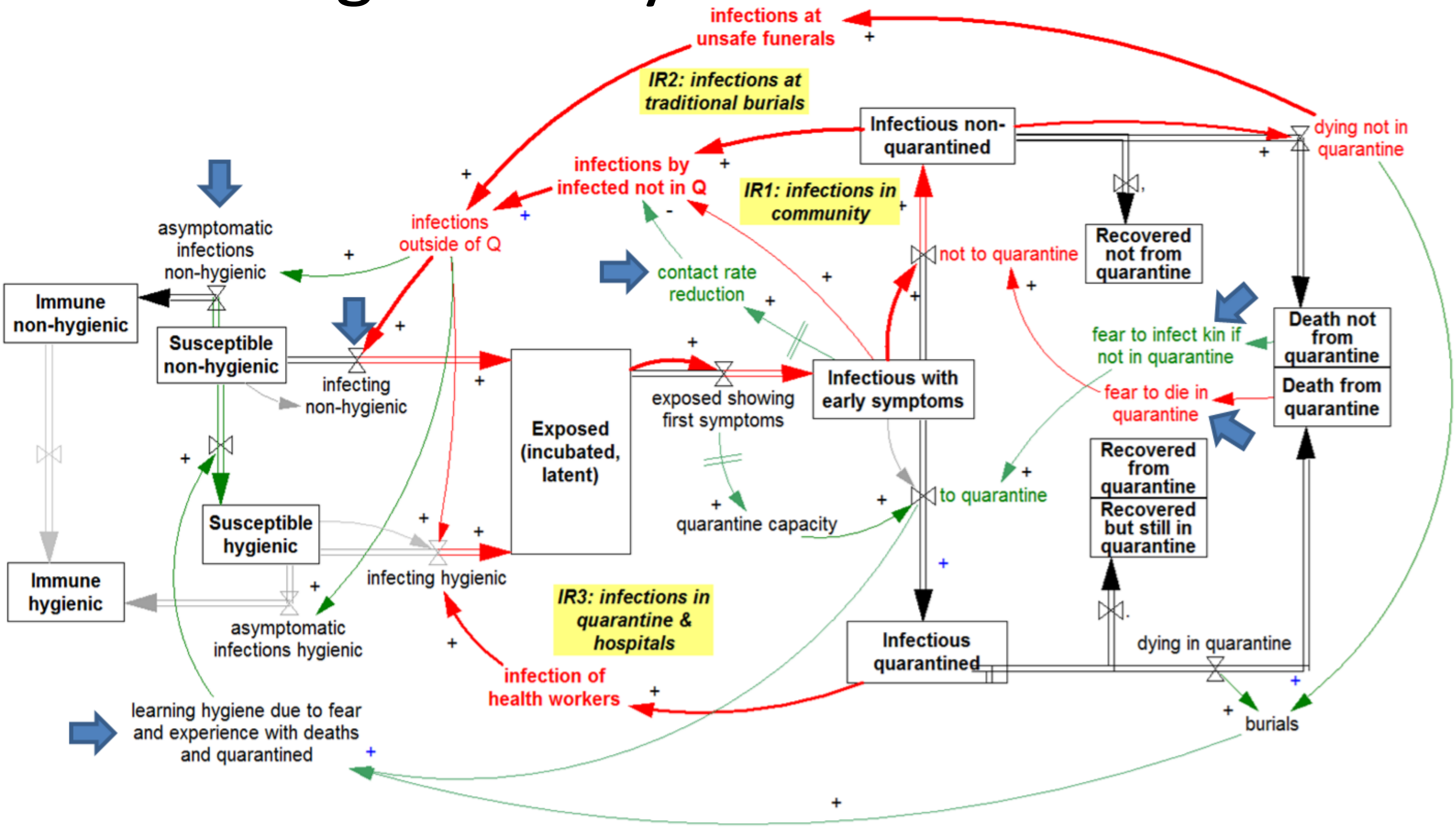
(d) Optimized Adaptive Policy

Pruyt & Hamarat 2010

- ExampleFluWithPoliciesV.ipynb
- PrimFlu.ipynb

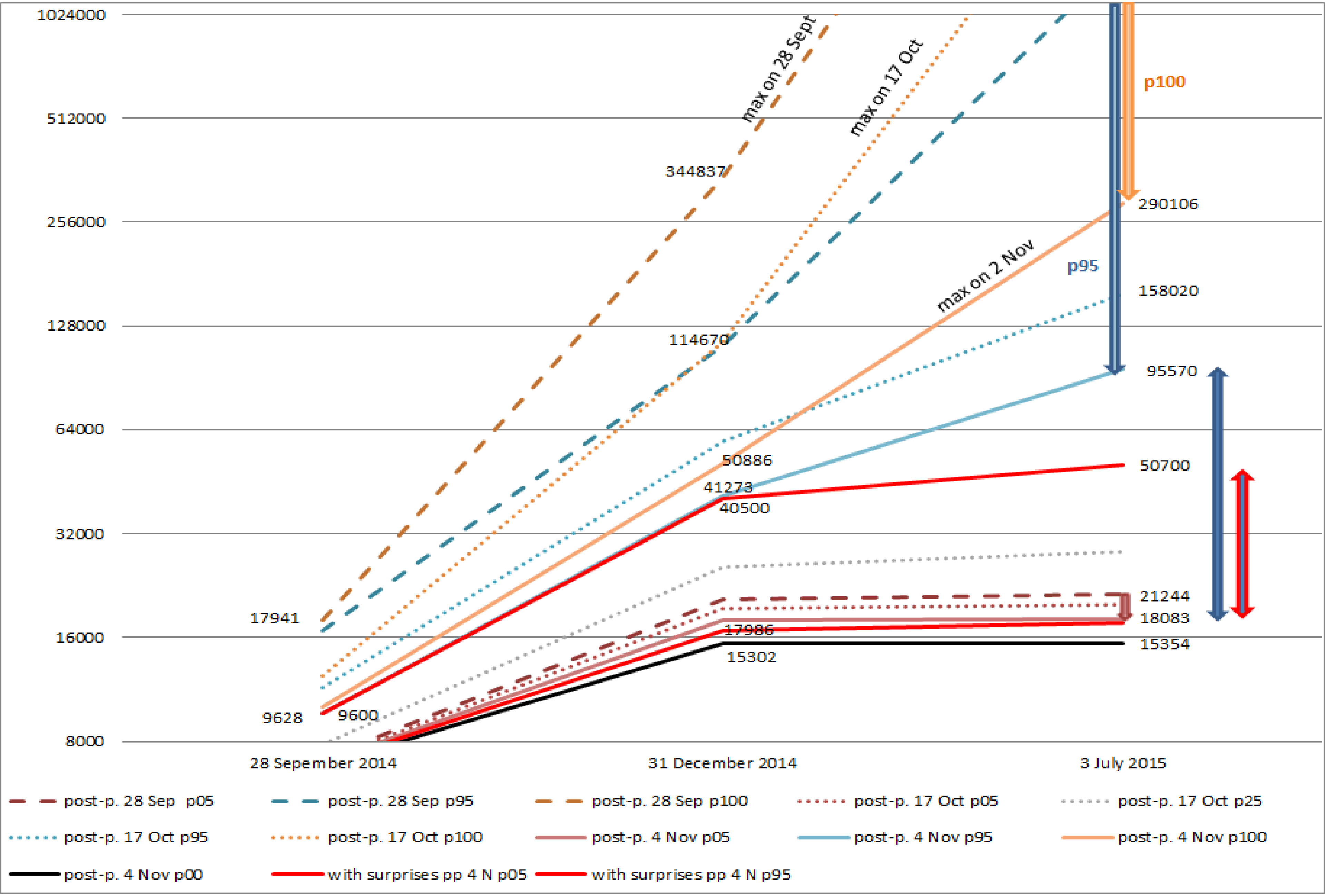


Example 2: Ensemble Forecasting and Testing of Policy Robustness - Ebola



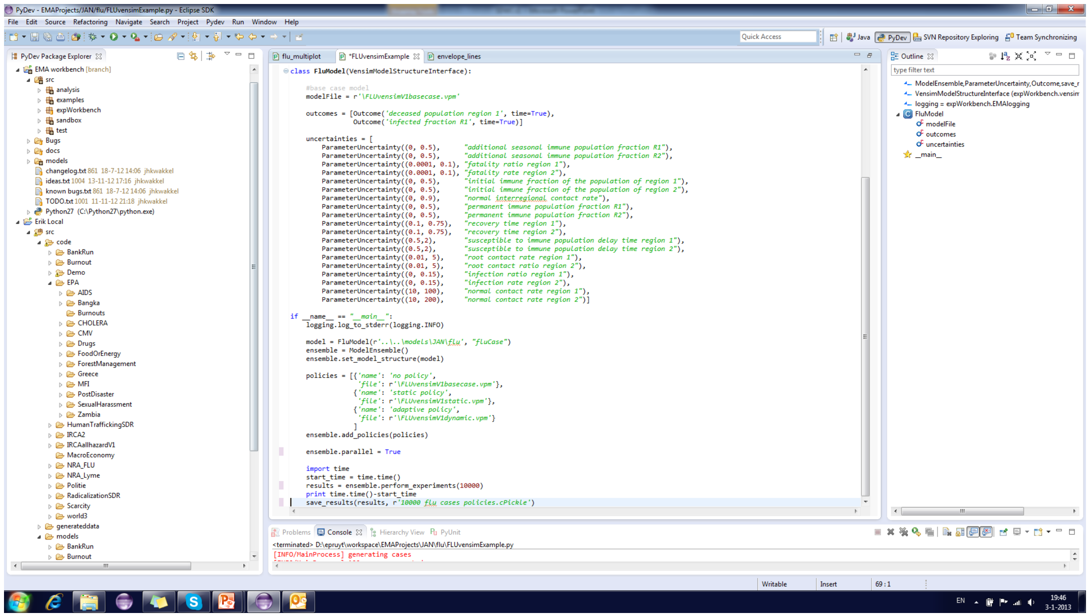
For some of our Ebola studies, see: Pruyt *et al.*, 2015. *Systems Research & Beh. Science*

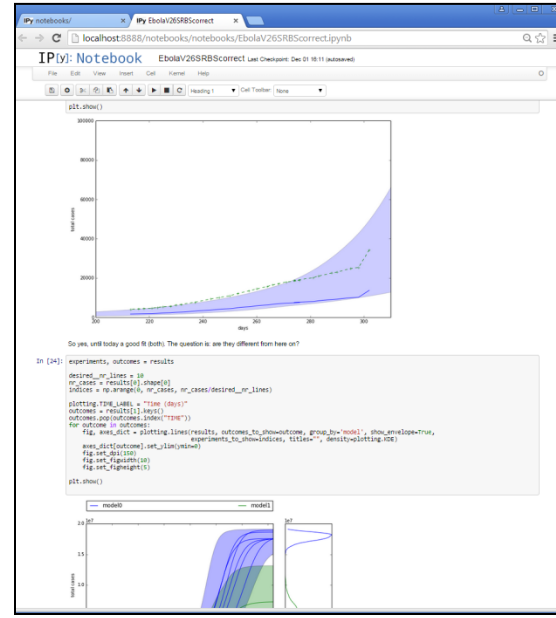
As well as: Auping *et al.*, 2016. *International Journal of Systems Science*



1024000
512000
256000
128000
64000
32000
16000
8000
max on 28 Sept
max on 17 Oct
max on 2 Nov
p100
p95
344837
114670
290106
158020
95570
50886
41273
40500
50700
17941
9628
9600
21244
18083
17986
15302
15354
28 September 2014
31 December 2014
3 July 2015
post-p. 28 Sep p05
post-p. 28 Sep p95
post-p. 28 Sep p100
post-p. 17 Oct p05
post-p. 17 Oct p25
post-p. 17 Oct p95
post-p. 17 Oct p100
post-p. 4 Nov p05
post-p. 4 Nov p95
post-p. 4 Nov p100
post-p. 4 Nov p00
with surprises pp 4 N p05
with surprises pp 4 N p95

- EbolaV26Models123456wPOLSprimmedV03_overtimeD291UncRed.py

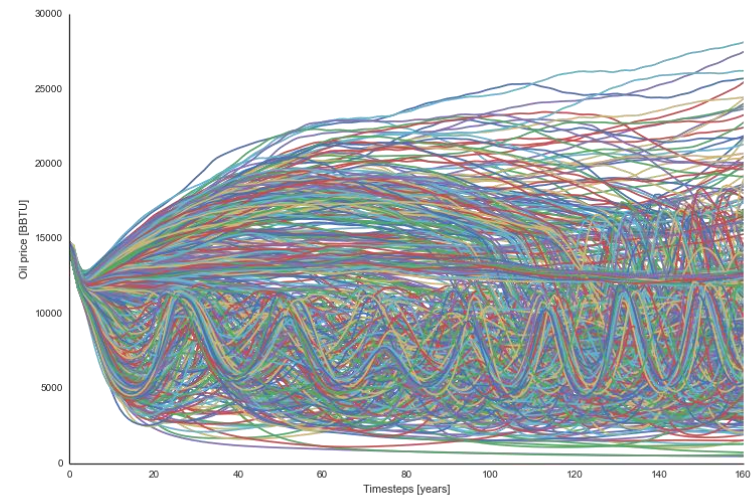




- + jupyter notebook
  - Soft calibration with PRIM
  - Postprocessing
  - Plotting of ensembles (different policies)
  - PRIM to identify what works / does not work
  - …

Adaptive Sampling: Why? What?

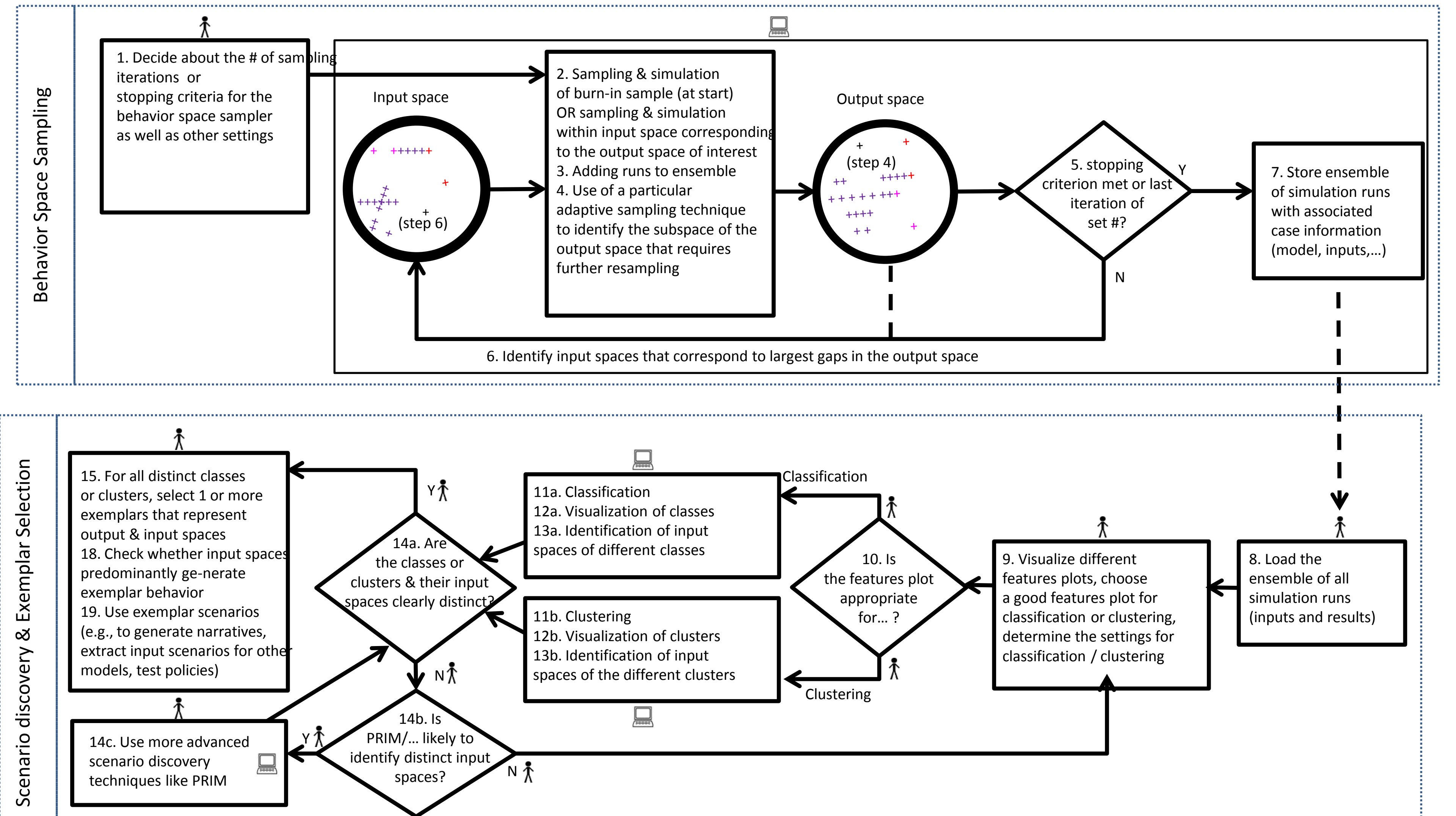
- What-if: really non-linear?
- Monte-Carlo? Latin Hyp?
- Sample, map, ID, resample



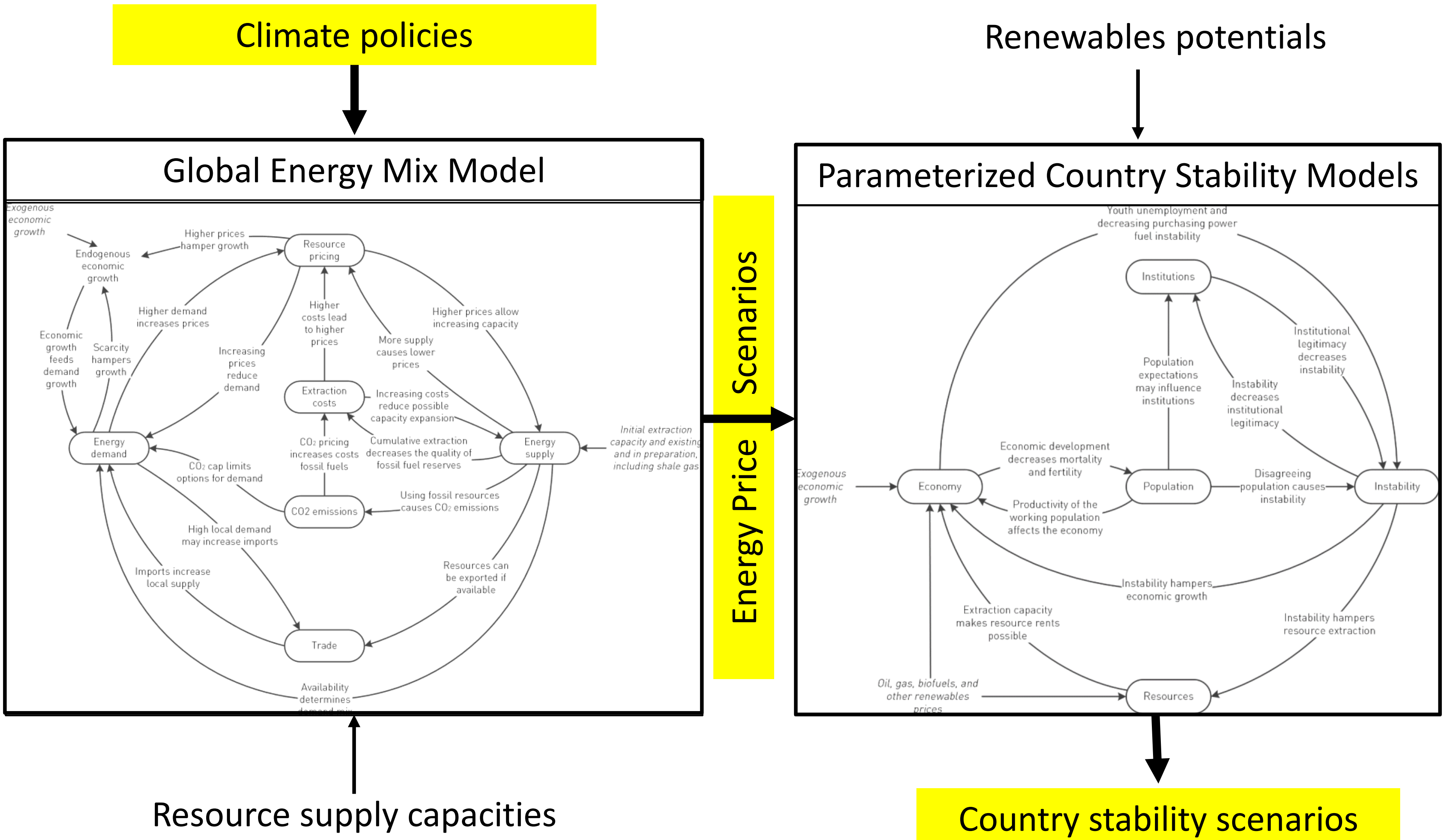
- For:
  - Scenario selection and narrative building
  - Scanning the spectrum of behaviours
  - Scanning the spectrum of policies without resistance
  - Identifying robust policy portfolios
  - Discovering surprising behaviours & corresponding input space

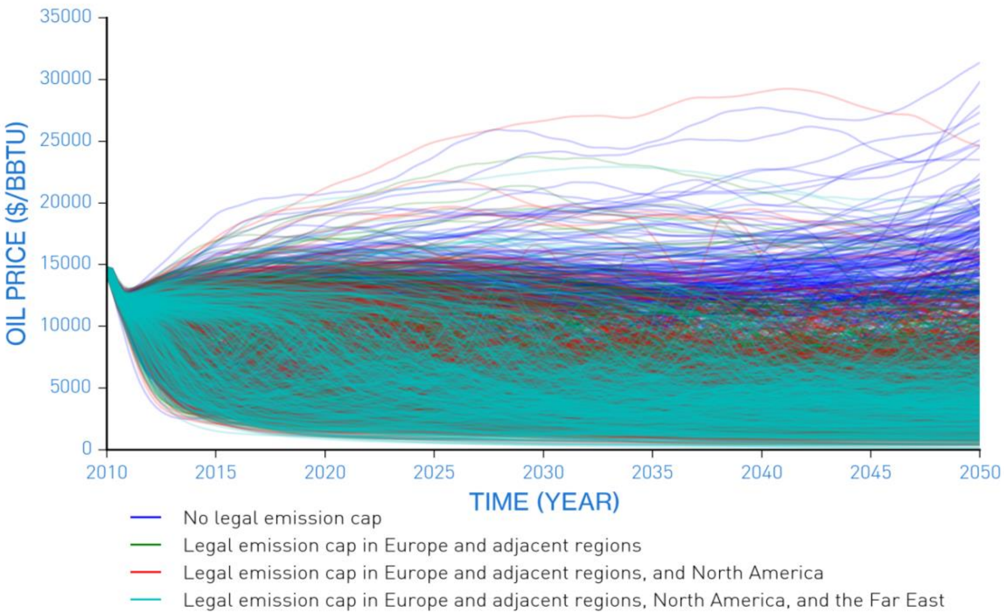
How? Identifying (Surprising) Behaviours?

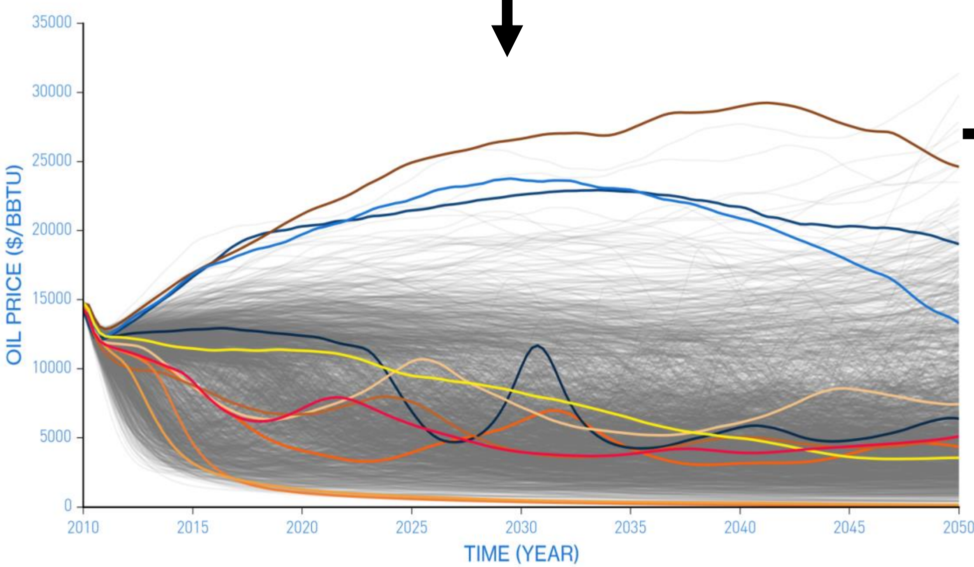
Behaviour Space Sampling + Behaviour-based classification/clustering + Input space identification & exemplar selection (Pruyt Islam 2016 SDR)

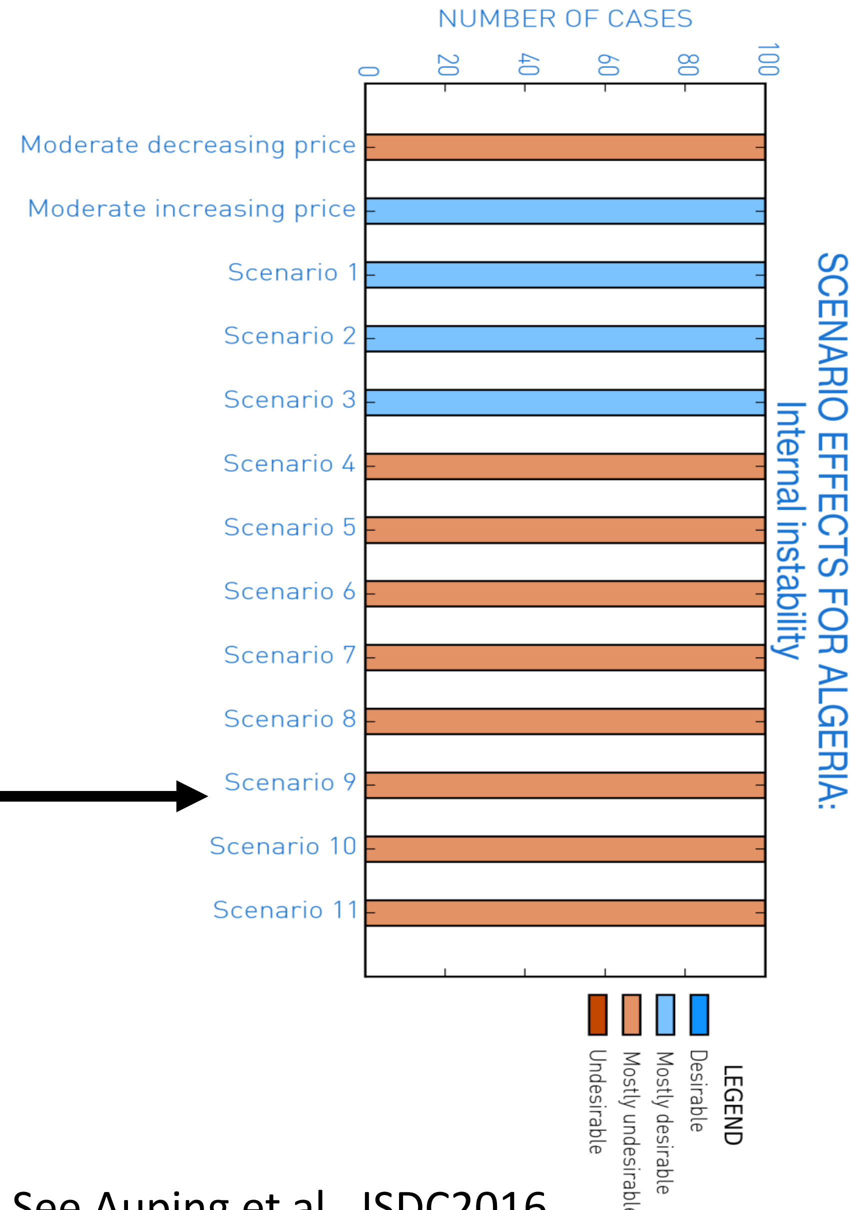


Example 1: Subset of Scenarios/Runs from Model 1 to Model 2, under Deep U.

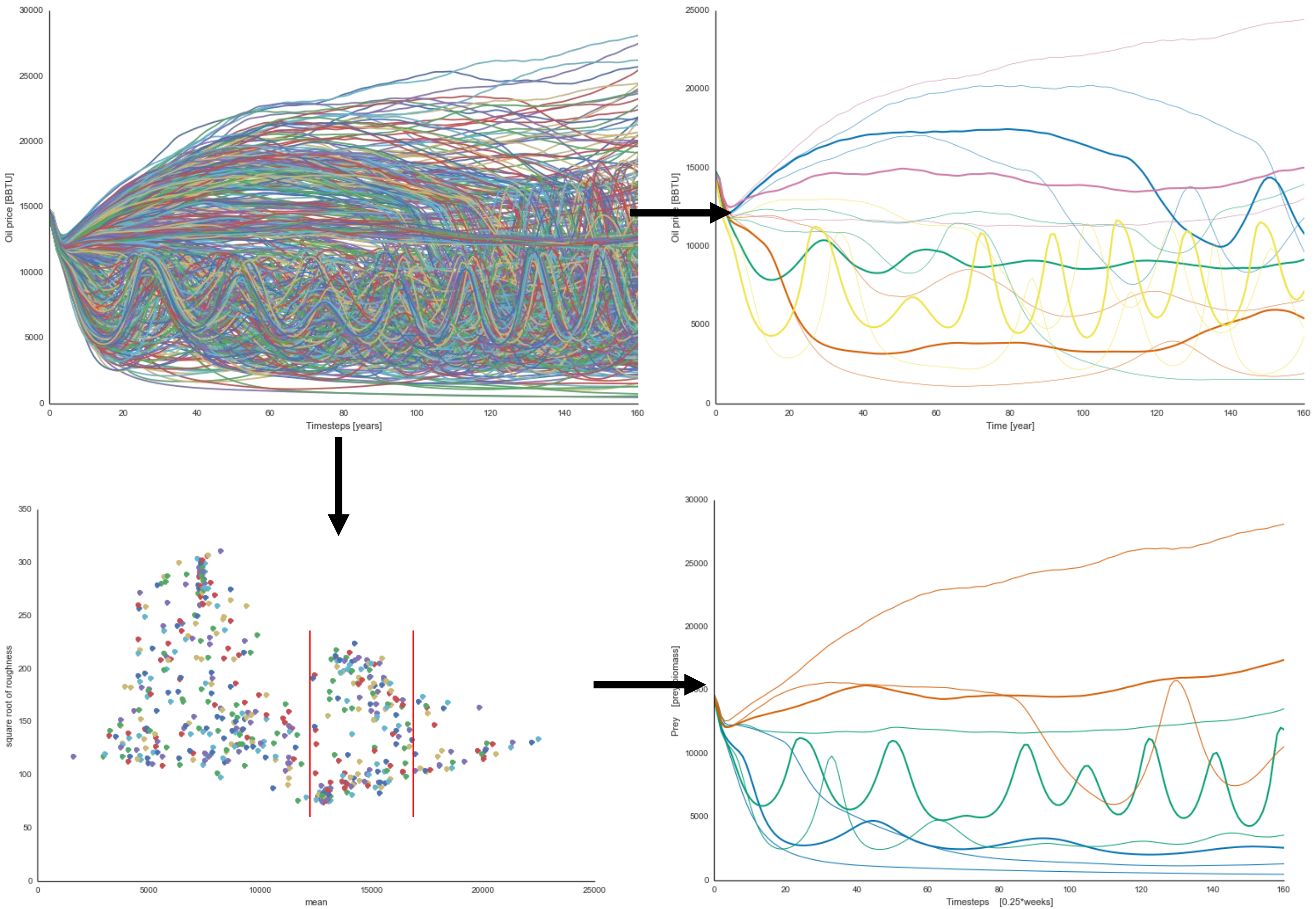








See Auping et al., ISDC2016



Oil price [BBTU]
Timesteps [years]
Oil price [BBTU]
Time [year]
square root of roughness
mean
Prey [prey biomass]
Timesteps [0.25*weeks]

Example 2: Burnout

- BSSv02b_Burnout01short_v01.ipynb
- adp_july.py
- adp_anlys.py

3) PySD: From Vensim models to Python +…, Simulation & Analysis in Python

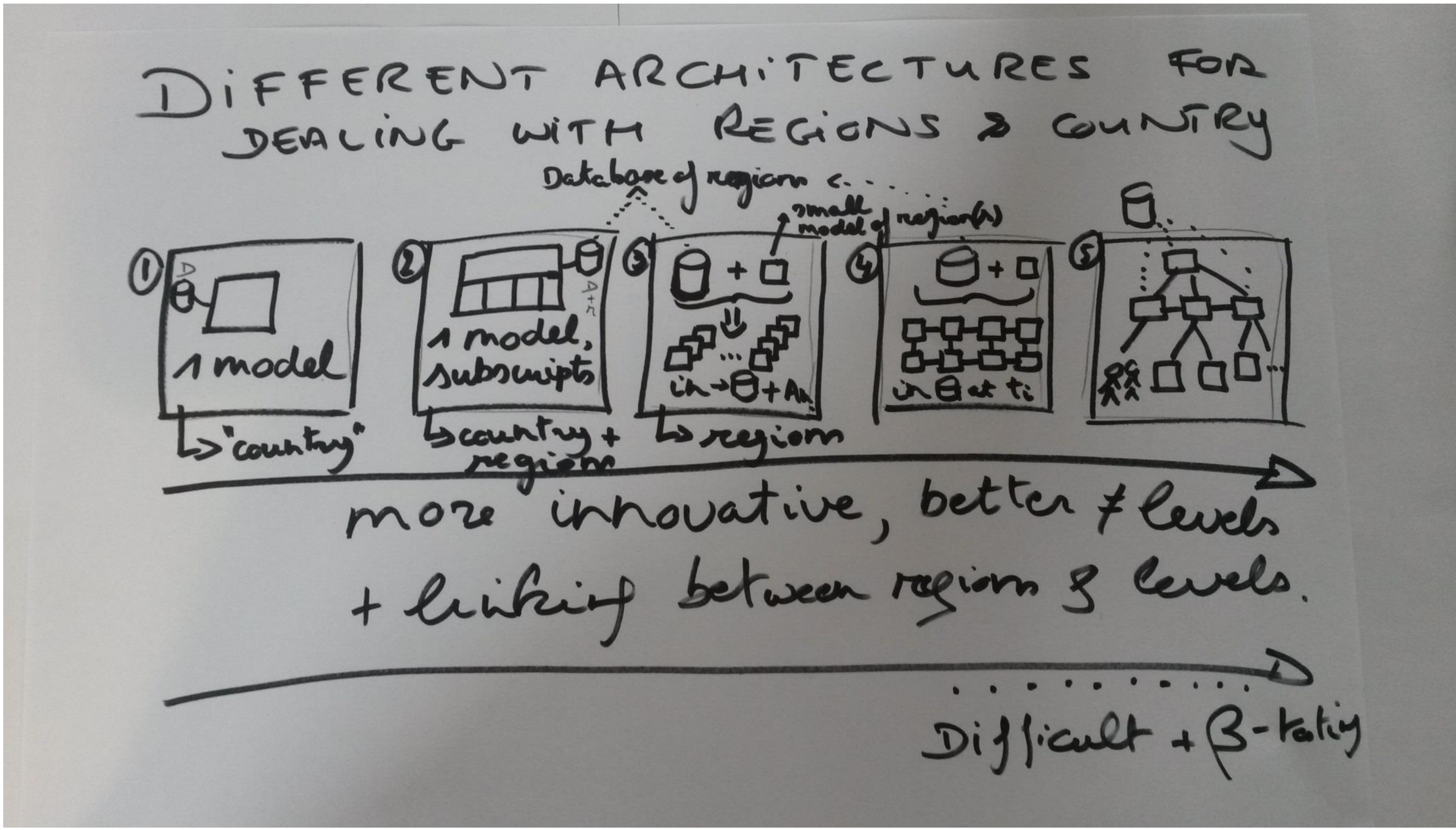
- Vensim: 2 make models, but fitting/plotting/…
- pySD: wrap Vensim model to python version
  - All python libraries become applicable
  - No need for Vensim DSS
  - No need for expensive computer: Raspberry Pi is enough
- Download pySD frm James Houghton’s Git Rep
- Source>analyses>
  - Getting_started
  - Fitting
  - …
  - Geo

4. From Aggregated to Disaggregated and Hybrid Modelling & Simulation

From 1 (subscripted) model as of old to:

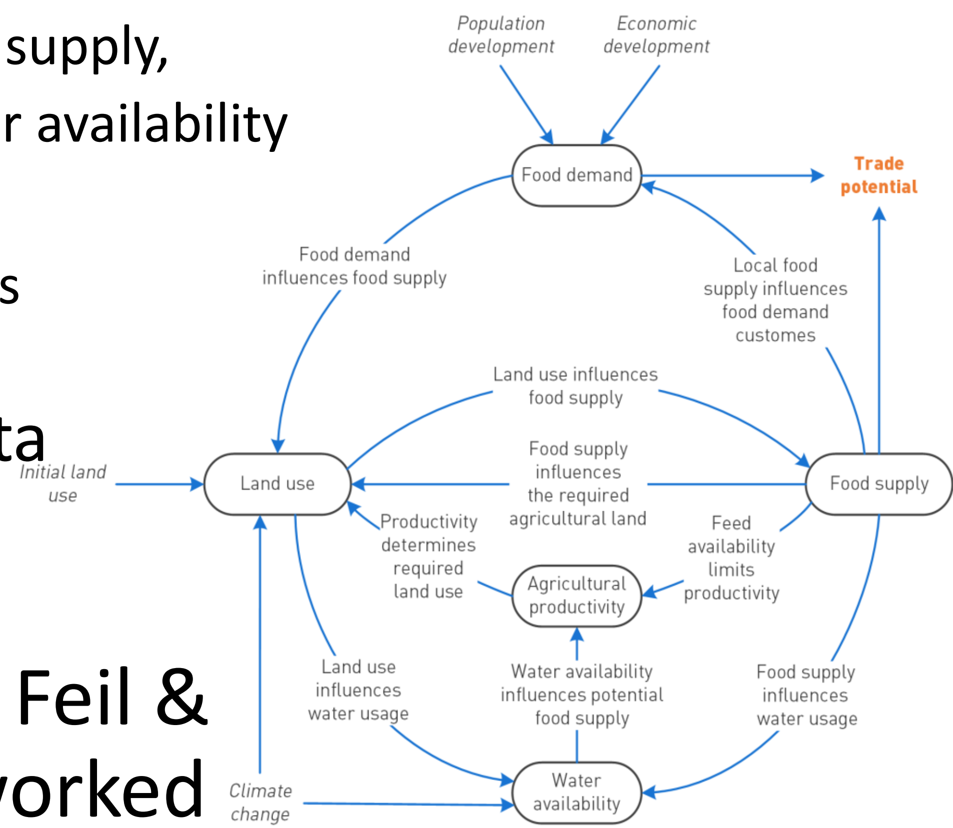
1. Simultaneous simulation of alternative models uU
   See: Pruyt & Kwakkel 2014 SDR; Pruyt et al 2015 SRBS;…
2. Subset of scen. runs from 1st model into 2nd model uU
   [Auping et al. ISDC2016, (JEPO)], (Pruyt Islam, '16 SDR)
3. Database + model(s) parameterized for many regions
   Without interaction btwn regions [see food study]
4. Database + parameterized model + interaction regions
   [see Schwarz Pruyt ISDC2016]
5. Layered geo-spatial model components x SD/AB/DES/
   [see Hesan Pruyt ISDC2016]

Or with a drawing



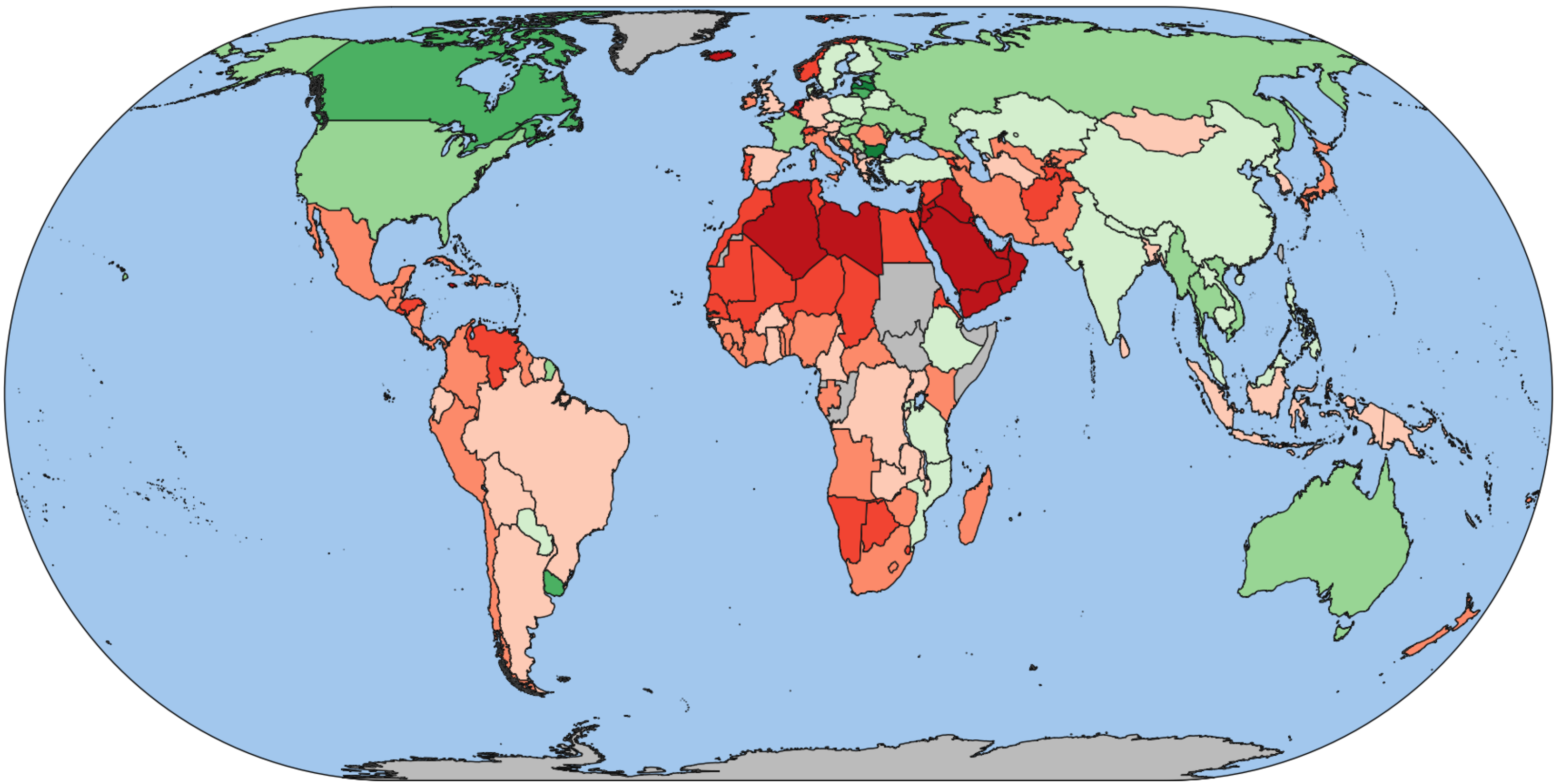
(3) Database + model parameterized for many regions (wo interaction)

- 1 model for food supply & demand per country
  - Five sub-models for
    - Food demand, Land use, Food supply,
    - Agricultural productivity, Water availability
  - 11 different food types, focus on 3: cereals, meat, & roots and tubers)
  - Large amount of input data
    - Data from FAOSTAT, UN pop. dept., IPCC,…
- For questions: Wouter Feil & Laurens de Kok have worked on this project (well done guys!)



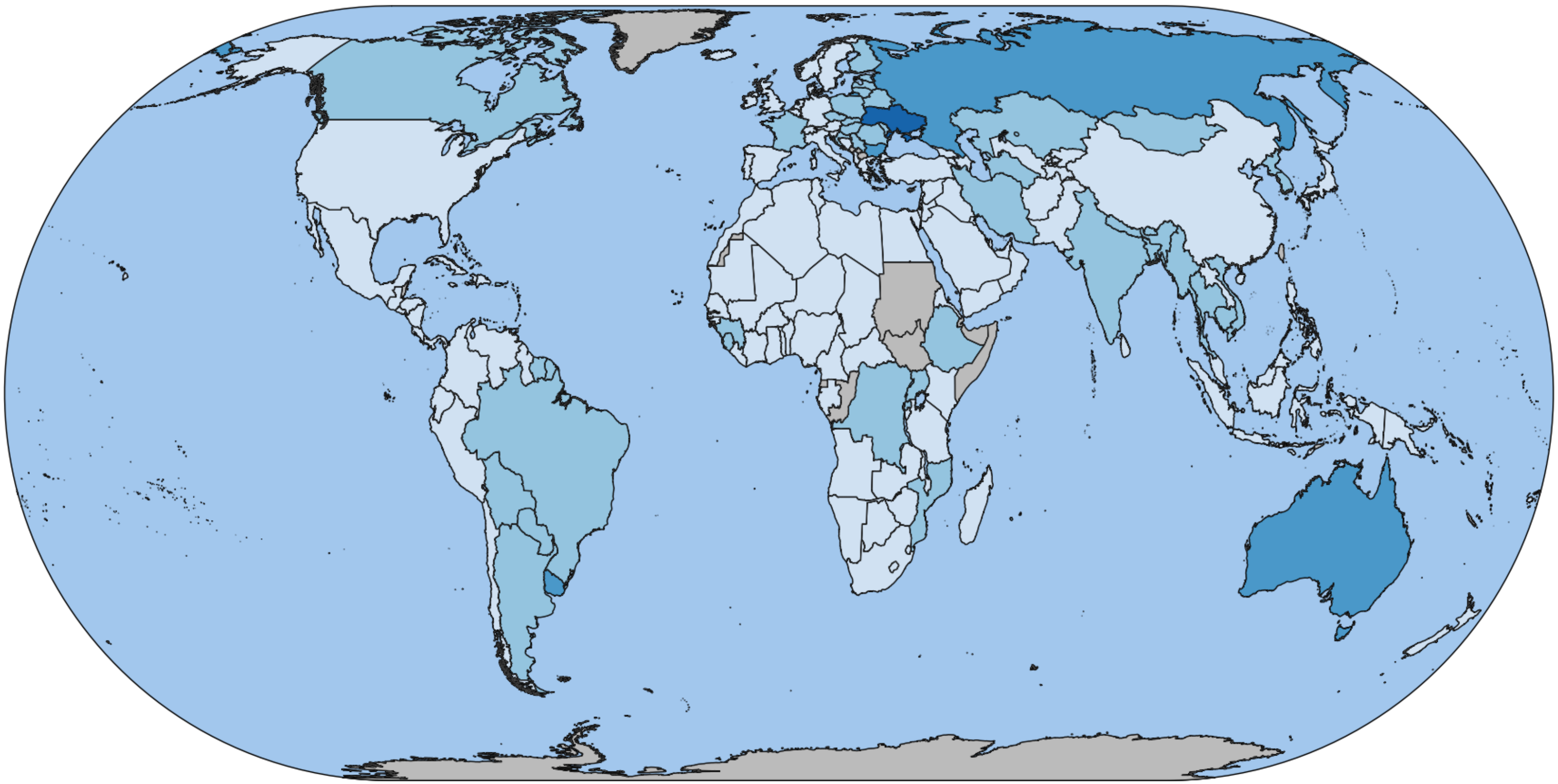
Descriptive statistics

RELATIVE TRADE POTENTIAL CEREALS 2031

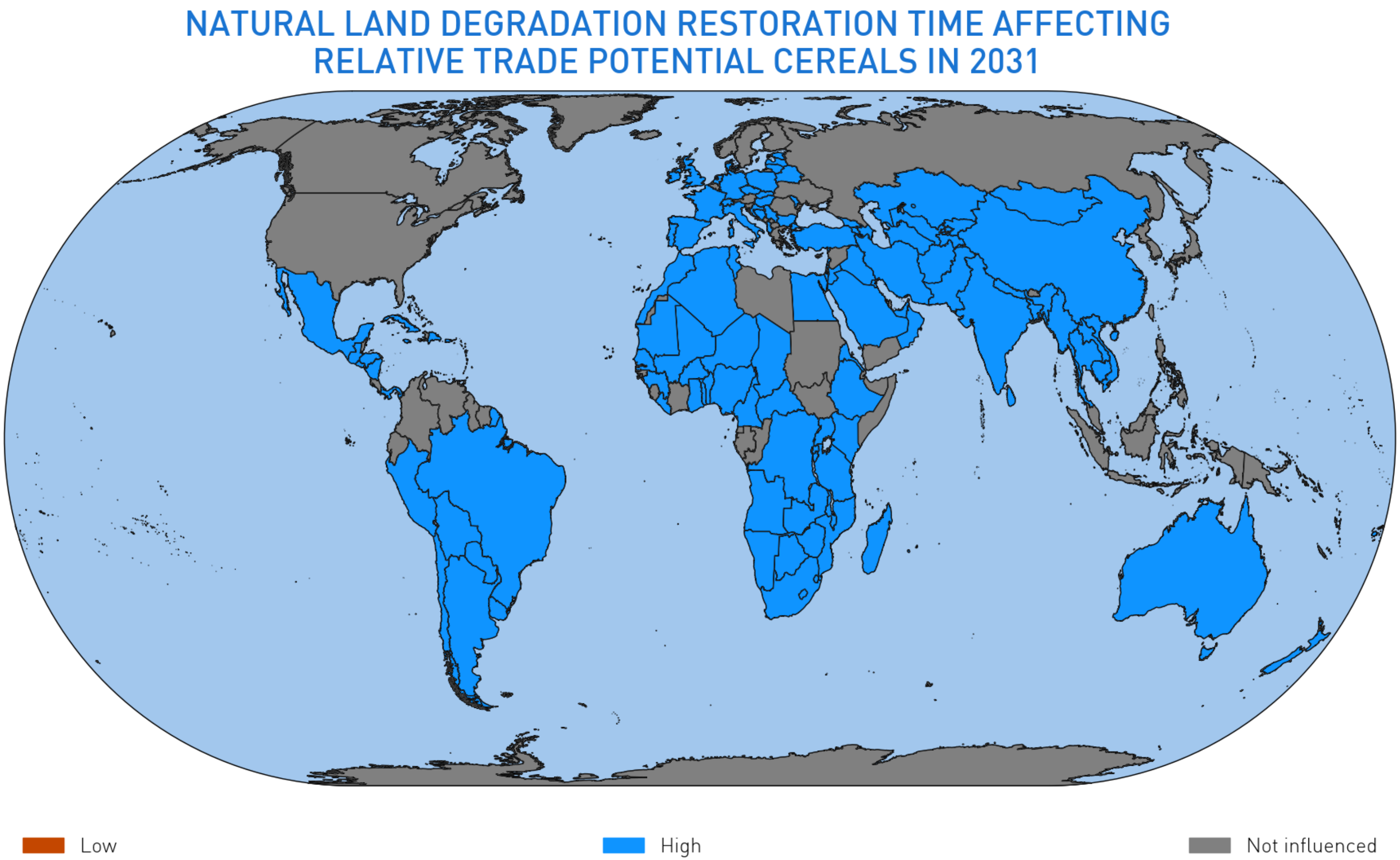


Uncertainty in outcomes

UNCERTAINTY IN RELATIVE TRADE POTENTIAL CEREALS 2031



PRIM: LAND DEGRADATION



(4) MSc thesis of Philipp Schwarz

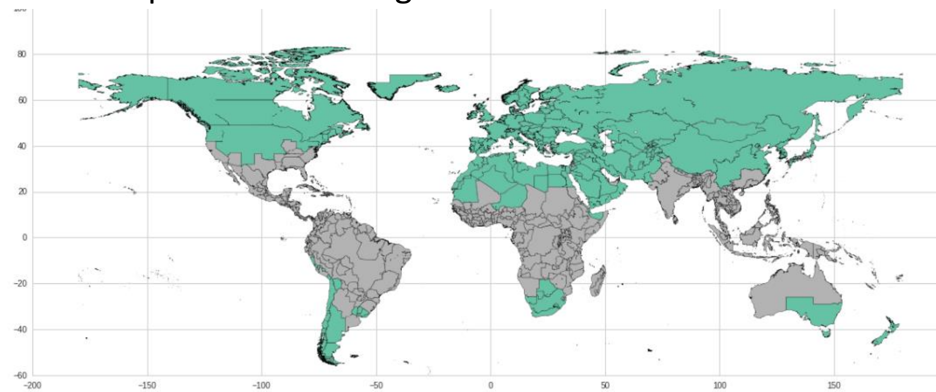
Collecting & using geo-referenced big data

Databases provided by Intergovernmental organization

THE WORLD BANK
Working for a World Free of Poverty

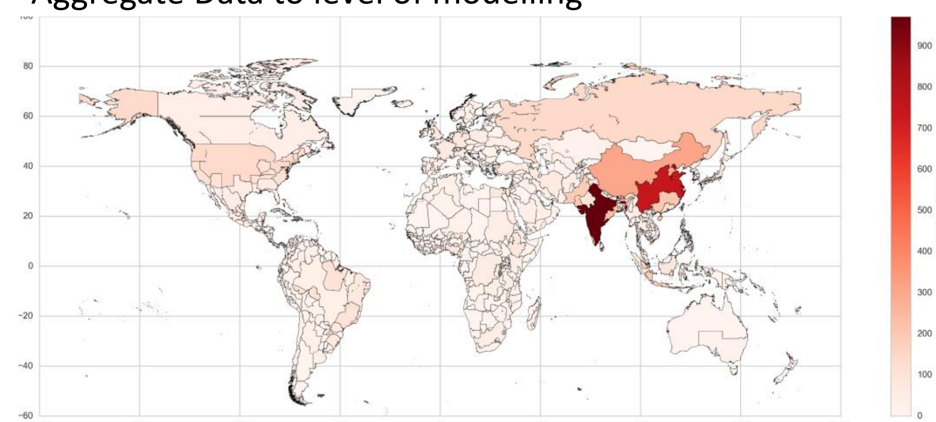
UNdata
A world of information

Data requirements on higher resolution than national-level



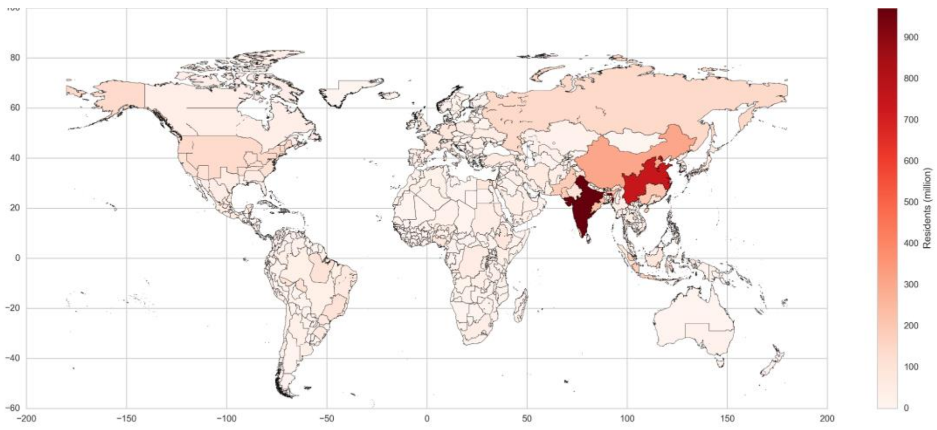
High-resolution gridded maps

Aggregate Data to level of modelling



CIESIN. 2015. “Gridded Population of the World, Version 4 (GPWv4): Population Count Adjusted to Match 2015 Revision of UN WPP Country Totals.” Center for International Earth Science Information Network - CIESIN - Columbia University. NASA Socioeconomic Data and Applications Center (SEDAC). http://dx.doi.org/10.7927/H4PR7SX1.

Data on the level of modelling



+ data from other modeling studies:

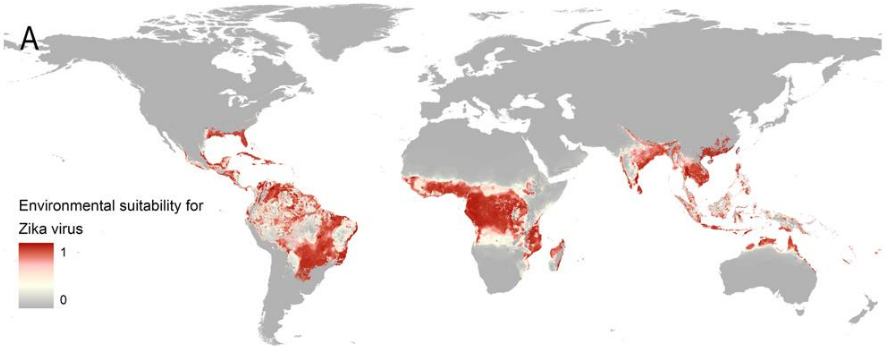
Model of global interconnectedness

Gravity Model of monthly global passenger air travel.
Based on socio-econ. of two places and their distance

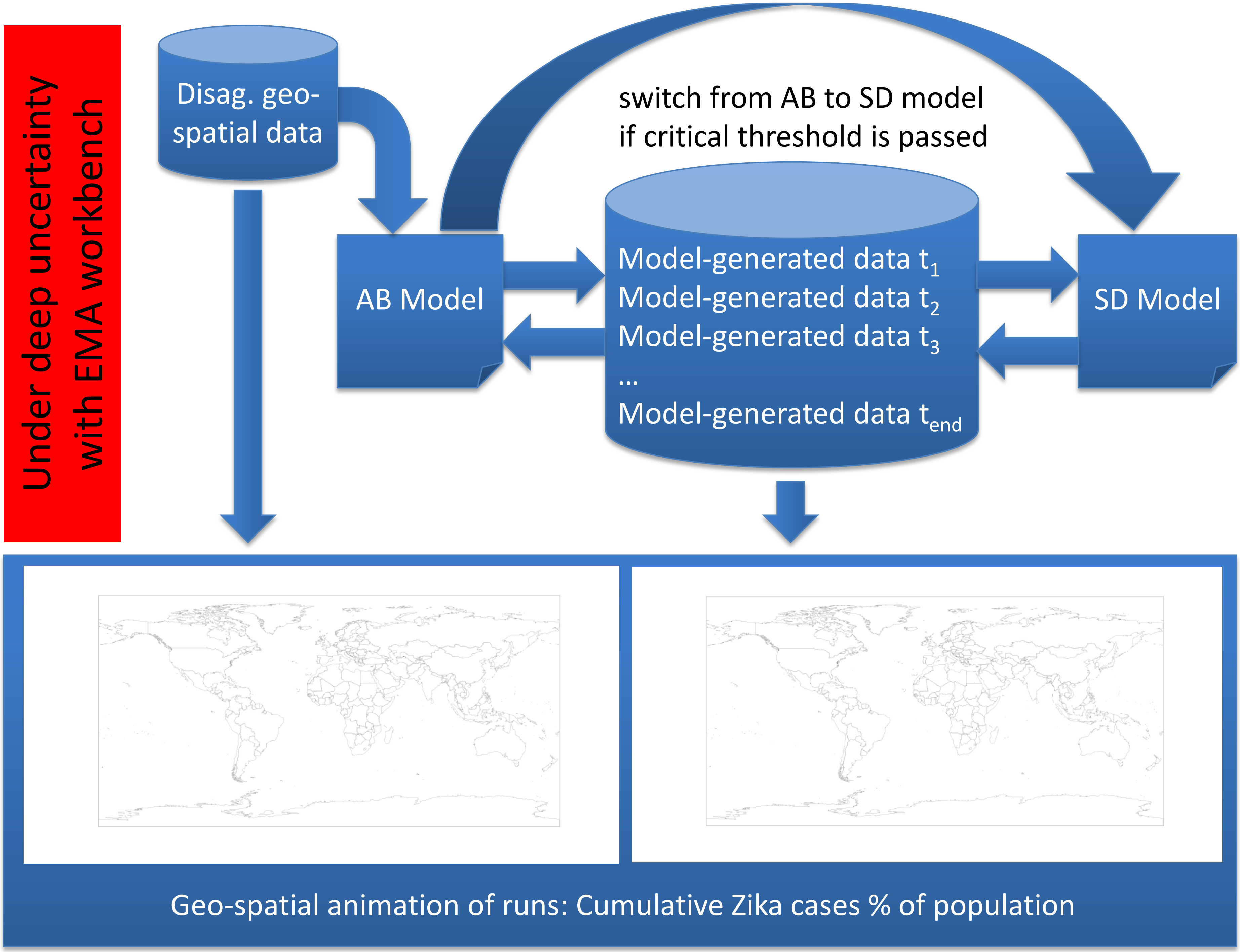
Mao, L., Wu, X., Huang, Z., Tatem, A.J., 2015. Modeling monthly flows of global air travel passengers: An open-access data resource. J. Transp. Geogr. 48, 52–60. doi:10.1016/j.jtrangeo.2015.08.017

Species Distribution GIS Model

Complex multivariate spatial relation between observations of species occurrence and environmental conditions



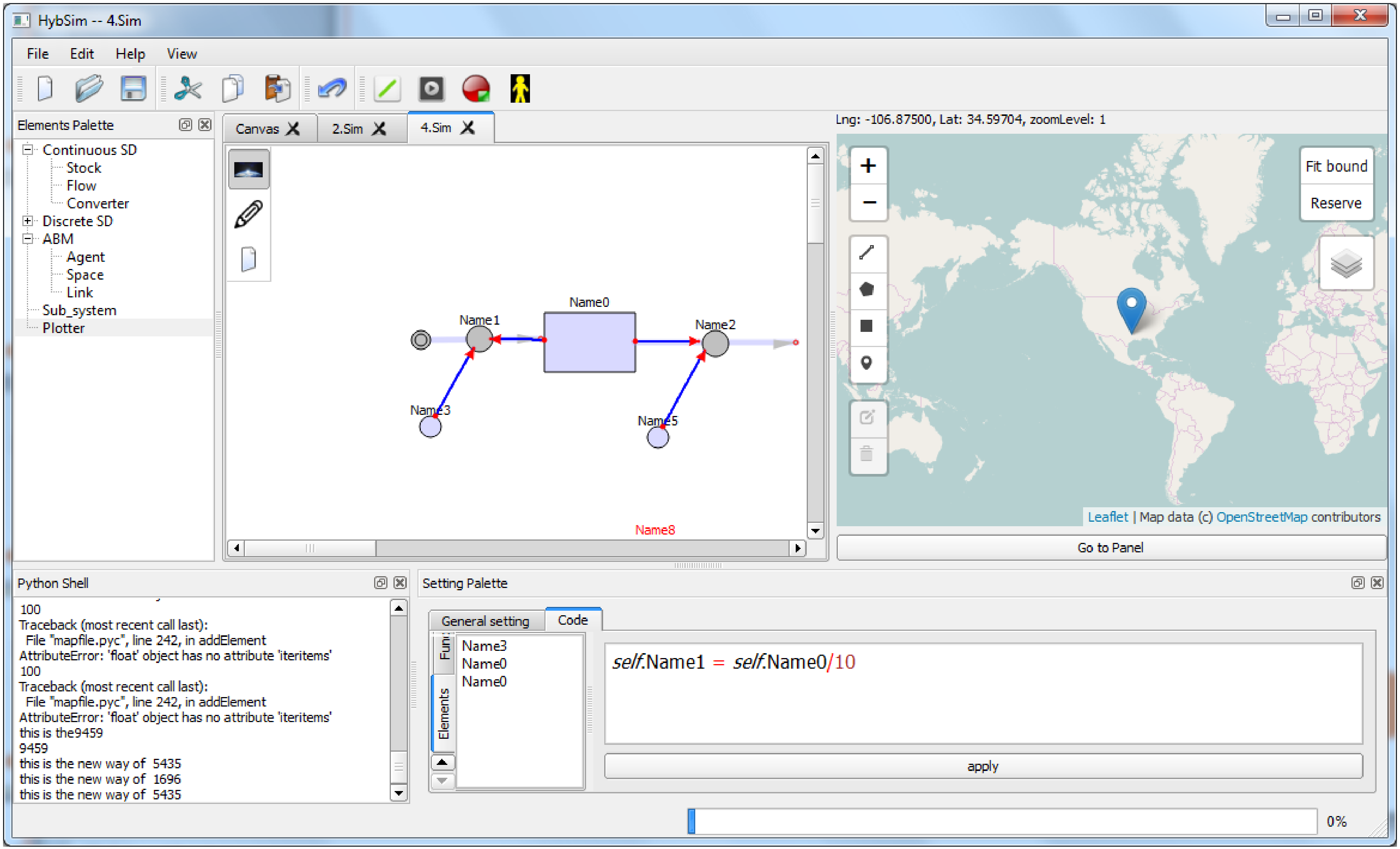
Messina, J. P. et al. (2016). Mapping global environmental suitability for Zika virus. eLife 5, e15272 [Data set] Requested from authors. https://elifesciences.org/content/5/e15272


Under deep uncertainty
with EMA workbench
Disag. geo-
spatial data
switch from AB to SD model
if critical threshold is passed
AB Model
Model-generated data t_1
Model-generated data t_2
Model-generated data t_3
…
Model-generated data t_{end}
SD Model
Geo-spatial animation of runs: Cumulative Zika cases % of population

Setting up database-driven simulations for a lower level of aggregation

- Raspberry Pi
- Philipp Schwarz’s Master Thesis (2016)
- Python code:
  - For making databases
  - Data handling and stacking
  - Switching between ABM and SD
  - Simulation under deep uncertainty
  - Analysis of results

(5) Hierarchical geo-spat. SD-ABM-DES M&S in Anysim [beta-version]



(6) The Full Monty [Python]?

- Complex models: Everything in python?
- See Bas Keijser’s Master Thesis:
  - SD x ABM x Oligopolistic market handling
  - Statistical analyses
- “Best graduate” competition on Nov 17!

Conclusions

- Python greatly enhances modelling and simulation!

$\Rightarrow$Database structures (into and out of)

$\Rightarrow$Scripting to force programs what to do

$\Rightarrow$Analytical tech (eg BS Sampling, Clustering, ML,…)

$\Rightarrow$Visualization of the results: on spot plotting on a map

- Many recent and near-future innovations [needed]
  - Modelling under deep uncertainty + analysis
  - Hybrid and systems-of-systems modelling
  - Database-driven / geo-spatial simulation
  - Visualizations and animations: “dynamic & on the map”

  + under uncertainty and on the spot in workshop settings