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Statistics for Complex Computer Models: Beyond Input-Output Analysis

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http://www.lanl.gov/orgs/tsa/tsa1/index.html

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- Andy Wolfsberg (Cl-36 work)

Outline

I. Introduction: TRANSIMS vs. a “traditional” computer model
II. Statistical simulation of model inputs
III. Model calibration
IV. Model assessment
V. Conclusions

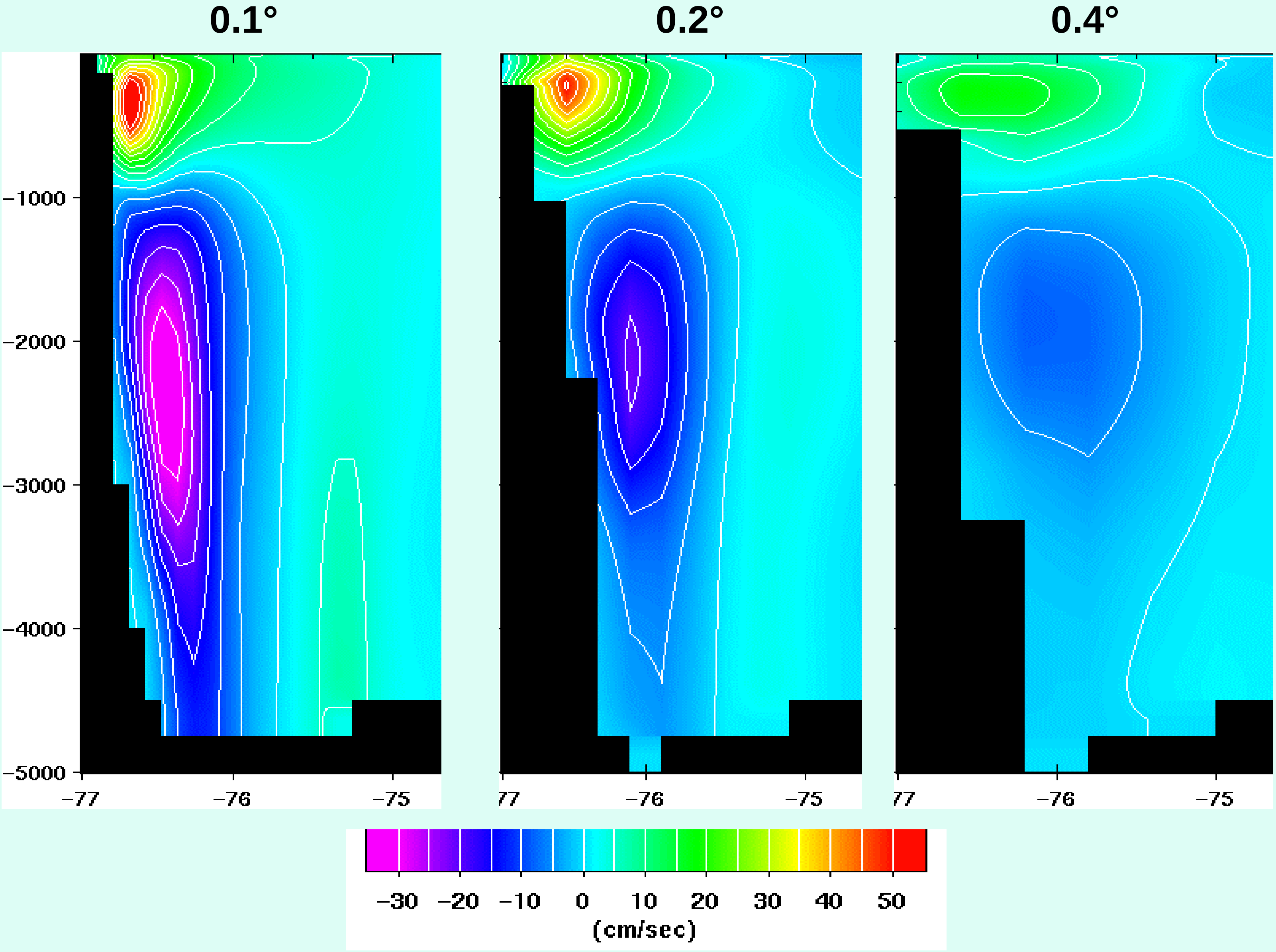
I. Complex computer models

- Dynamical
  - Some kind of process model
    - “Traditional”: Systems of differential equations
    - “Novel”: Cellular automata, sequential dynamical systems...
- Composed
  - Maybe on more than one scale
    - Very large ensembles of similar, locally interacting components
    - Coupling of several dissimilar components
- Large
  - Large fields of input parameters
  - Huge amounts of output
  - Ensemble dynamics less well understood

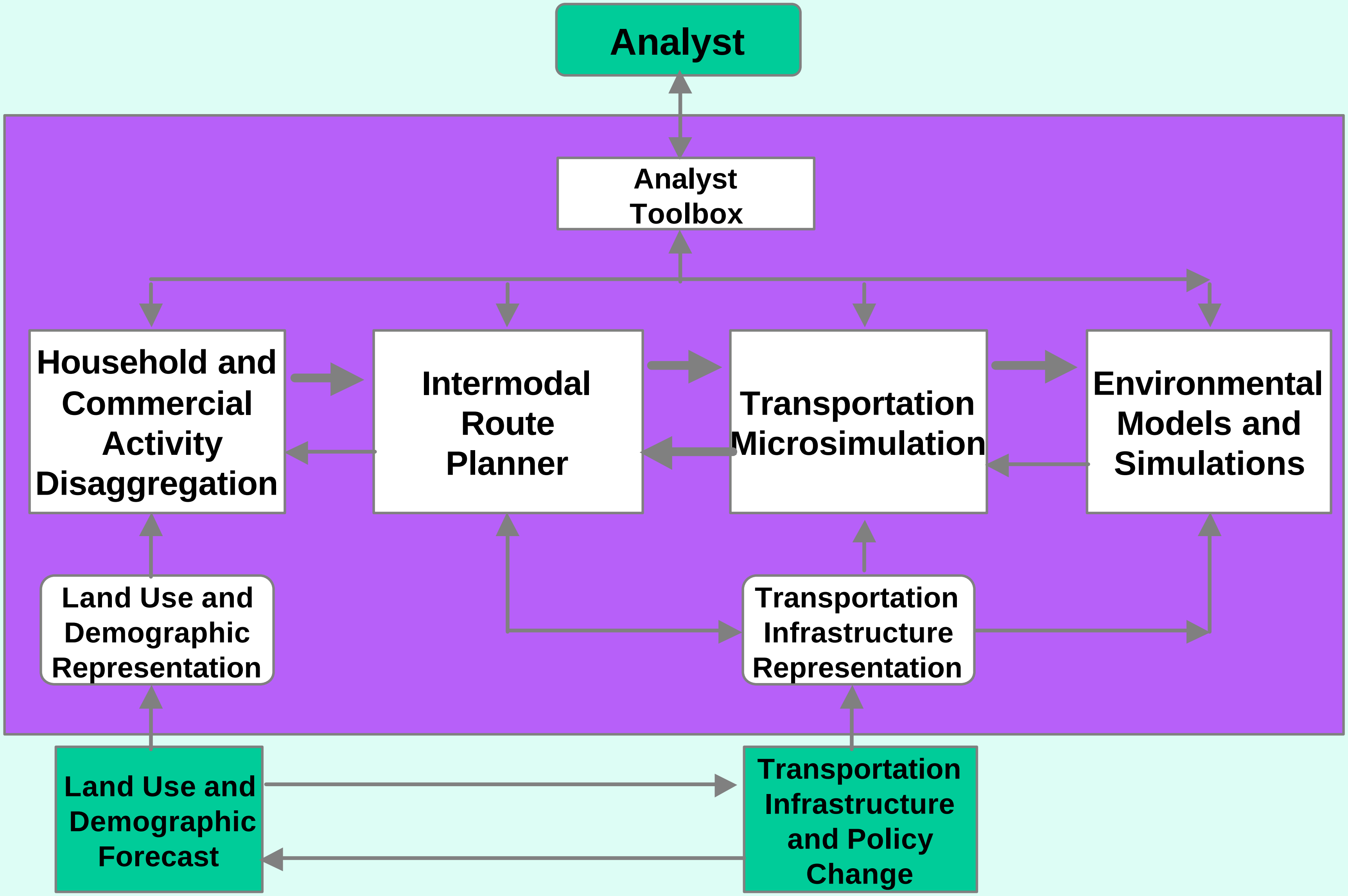
Requirements for ocean model

- Representation of dynamics: PDE system
- Boundary conditions
  - Basin topography (static)
  - Wind fields (dynamic)
- Calibration
  - Parameters of subgrid phenomena
  - Spin-up to initial conditions
- Assessment
  - Comparisons with satellite data (SSH for example)
  - Inspection

Meridional velocity at 26.5°N



TRANSIMS Architecture



Analyst

Analyst Toolbox

Household and Commercial Activity Disaggregation

Intermodal Route Planner

Transportation Microsimulation

Environmental Models and Simulations

Land Use and Demographic Representation

Transportation Infrastructure Representation

Land Use and Demographic Forecast

Transportation Infrastructure and Policy Change

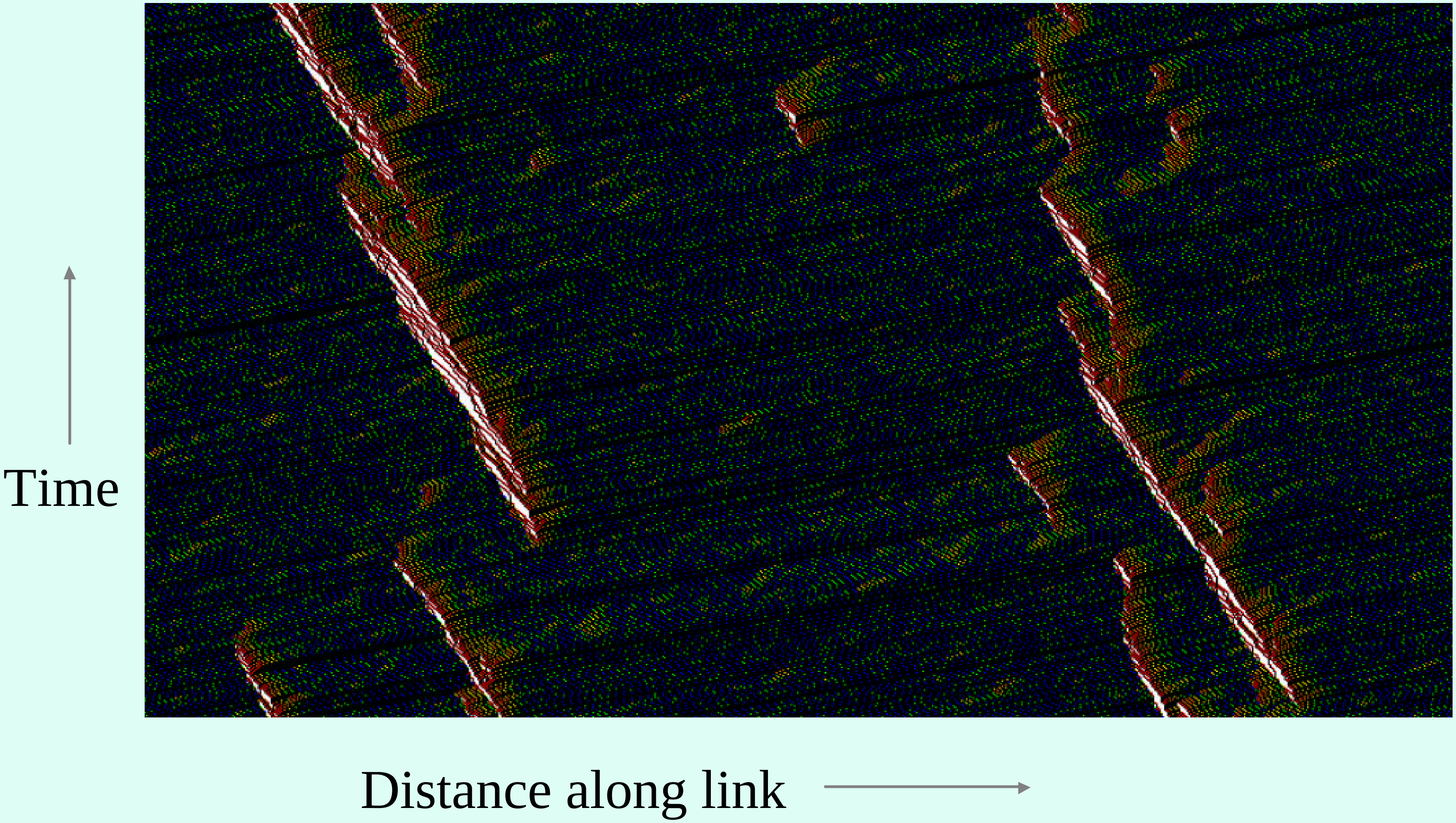
Modeling with TRANSIMS

- Representation of dynamics
  - Small-scale dynamics (microsimulation)
  - Ensemble dynamics (emergent)
- Boundary conditions
- Calibration
- Assessment

Cellular Automaton Driving Rules

- total of about twelve adjustable parameters for driving rules
- movement forward on grid based on gap to next vehicle, current speed, maximum speed
- lane changes based on chosen approach lane to next intersection, current speed, gap to next vehicle in current lane, gaps to previous and next vehicles in new lane
- intersection entry based on position and speed on link, occupancy of intersection buffer, state of oncoming and interfering traffic

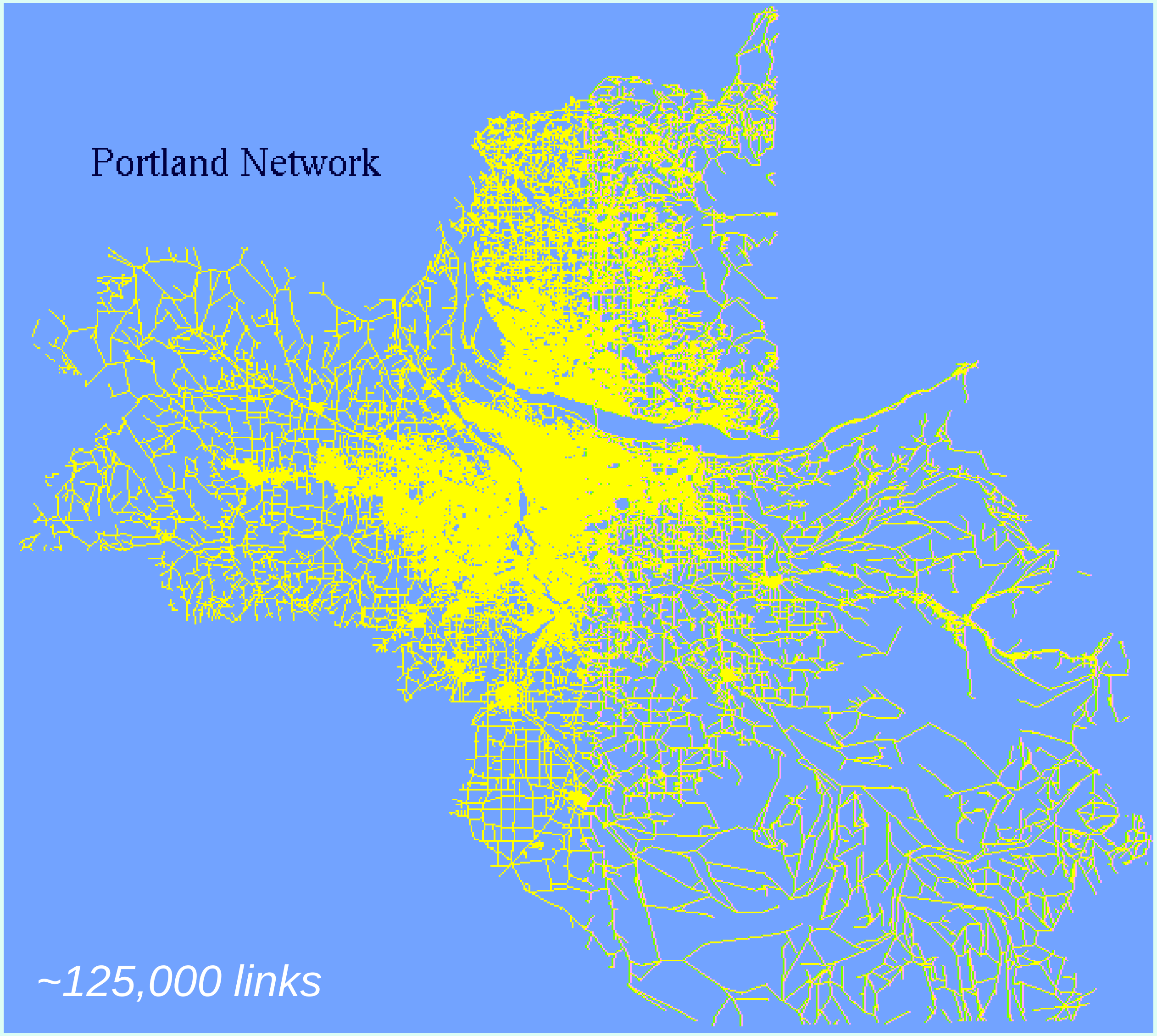
Example Vehicle Trajectories



II. Modeling with TRANSIMS: Boundary conditions

- Representation of dynamics
- Boundary conditions
  - Static conditions
    - Network, transit routes and schedules
  - Dynamic conditions
    - Realizations of population, demand
- Calibration
- Assessment

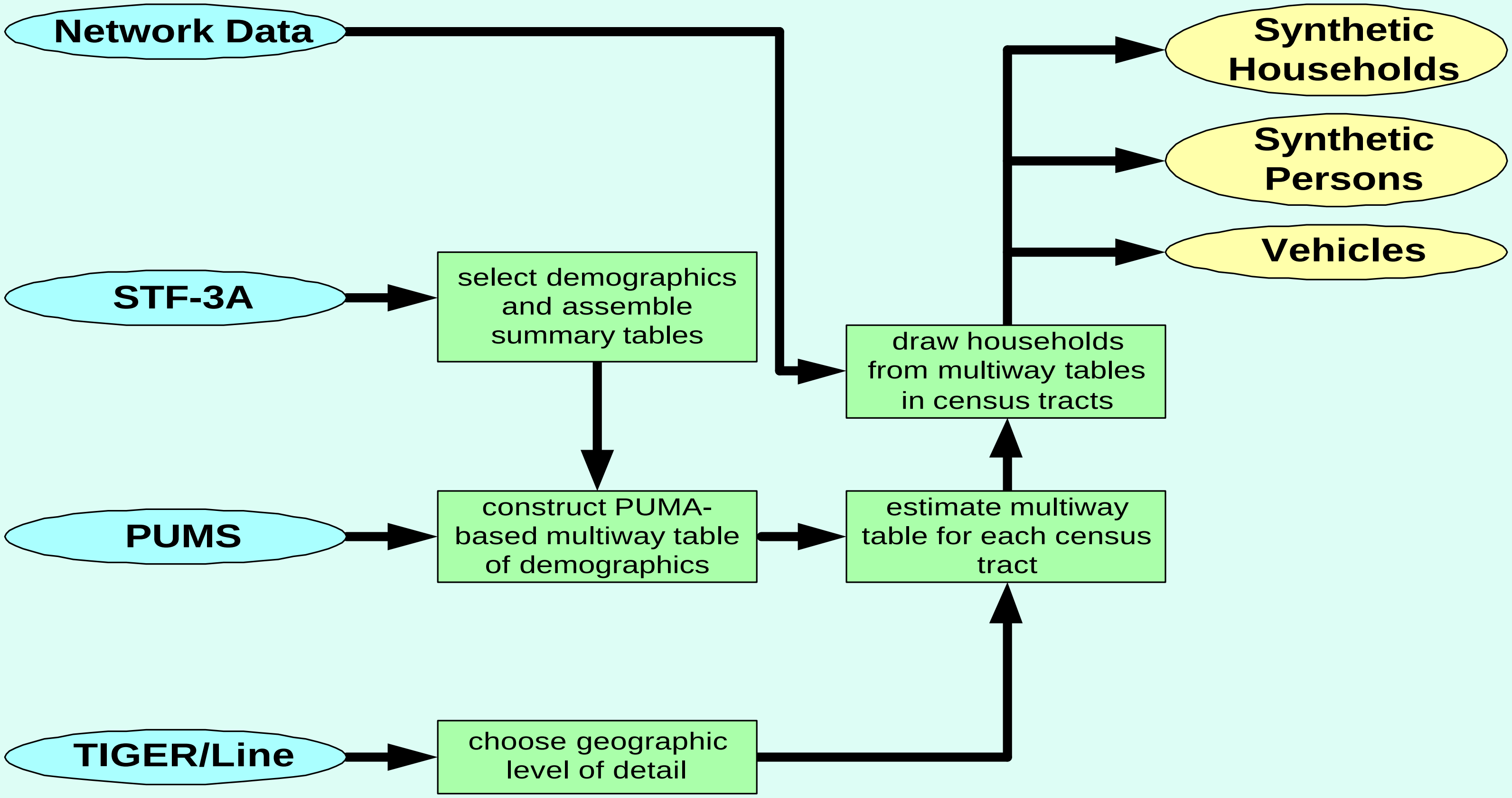
Example Network for Portland, Oregon



Population Synthesizer: Purpose

- creates a regional population realization...
  - demographics closely match real population
  - households are distributed spatially to approximate regional population distribution
- synthetic population’s demographics form basis for individual and household activities requiring travel
- household locations determine some of the travel origins and destinations

Population Synthesizer: Algorithm (Beckman, Baggerley and McKay 1996)



Network Data

STF-3A

PUMS

TIGER/Line

select demographics and assemble summary tables

construct PUMA-based multiway table of demographics

choose geographic level of detail

estimate multiway table for each census tract

draw households from multiway tables in census tracts

Synthetic Households

Synthetic Persons

Vehicles

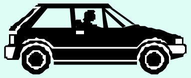
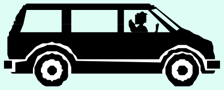
Population synthesizer: IPF steps

Contingency table	**Margins**	**RAKE'd estimate**
Weighted cross-classification of PUMS data by STF-3A marginal variables	Sums of STF-3A margins across census block groups in PUMA	"Average" table for PUMA
Table of ones with one more dimension than number of marginal variables	Individual block group margins plus the PUMA "average" table	Complete table for each block group in the PUMA
Weighted cross-classification of PUMS data by forecast variables	Individual block group margins for the forecast variables	Forecast table for each block group in the PUMA

🟩 Base year

🟦 Forecast year

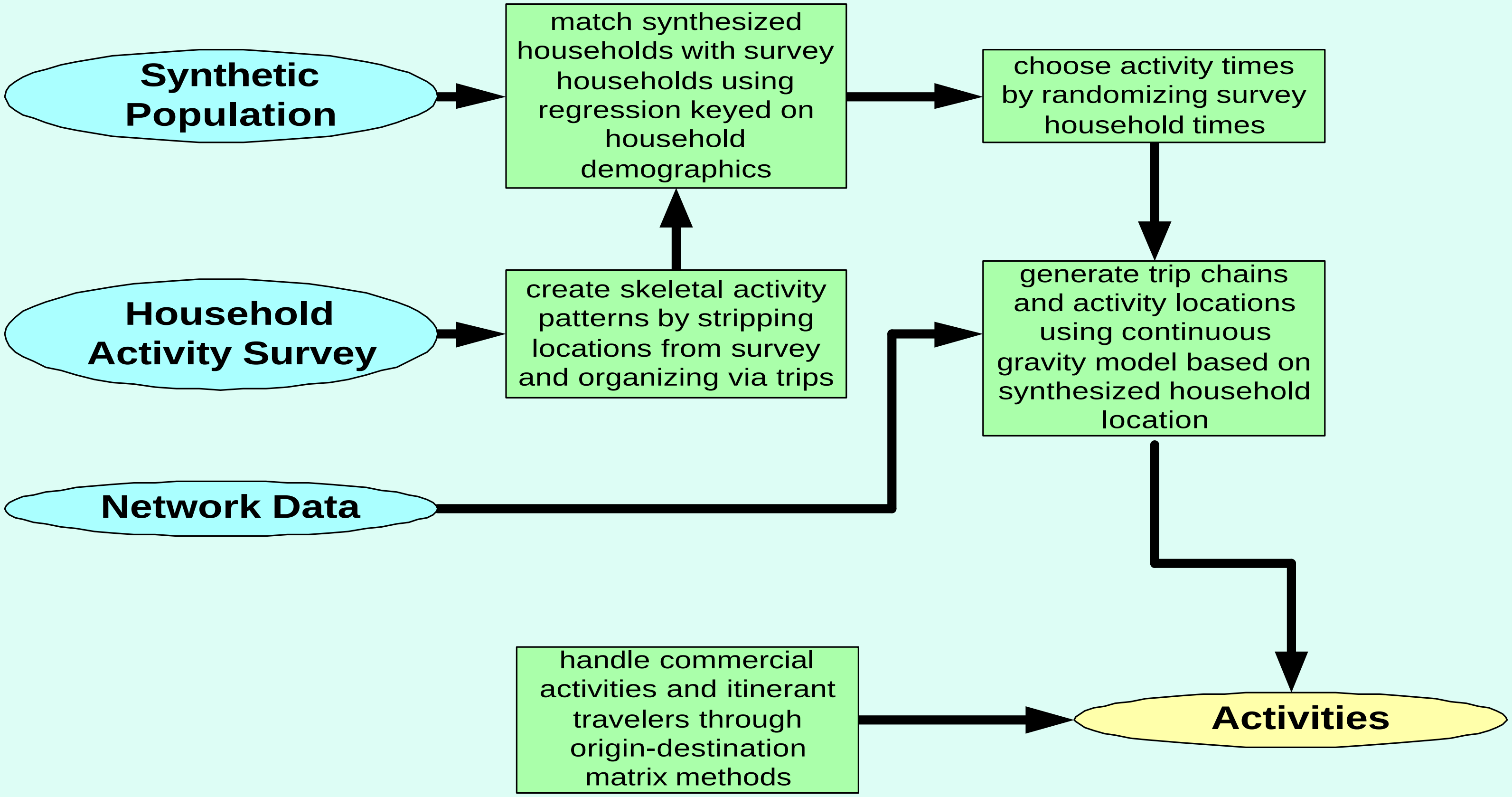
Example Household from PUMS in Portland, Oregon

Age	26	26	7
Income	$27k	$16k	$0
Status	worker	worker	student
Automobile			

Activity Generator: Purpose

- creates . . .
    - household and individual activities
    - activity priorities
    - activity locations
    - activity times
    - mode and travel preferences
- generates travel demand sensitive to demographics of synthetic population
- activities form basis for determining individuals’ trip plans for the region

Activity Generator: Algorithm (Speckman, Sun, Vaughn)



Synthetic Population

Household Activity Survey

Network Data

match synthesized households with survey households using regression keyed on household demographics

create skeletal activity patterns by stripping locations from survey and organizing via trips

choose activity times by randomizing survey household times

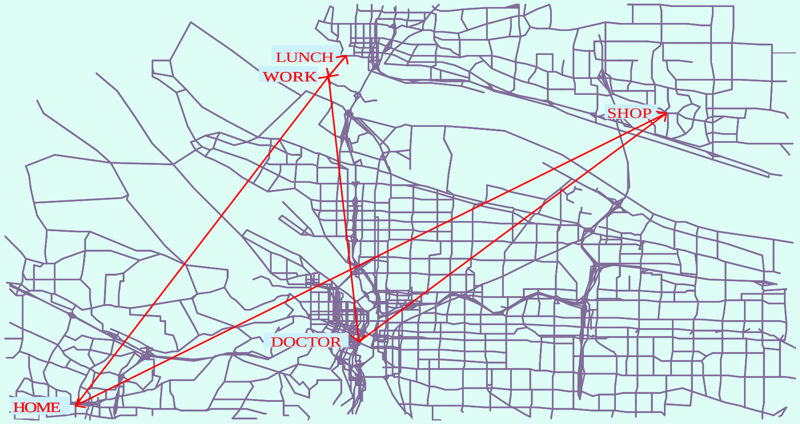
generate trip chains and activity locations using continuous gravity model based on synthesized household location

handle commercial activities and itinerant travelers through origin-destination matrix methods

Activities

Example Activities in Portland, Oregon

first person in household



second person in household

III. Modeling with TRANSIMS: Model Calibration

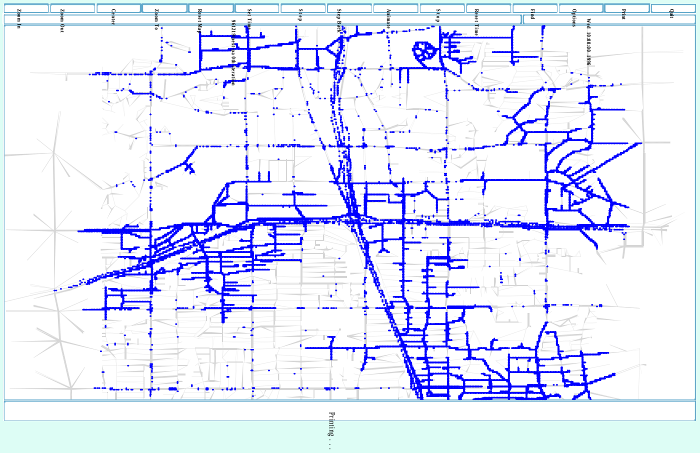
- Representation of dynamics
- Boundary conditions
- Calibration
    - Parameters in microsimulator
    - Initial conditions
    - Boundary conditions
- Assessment

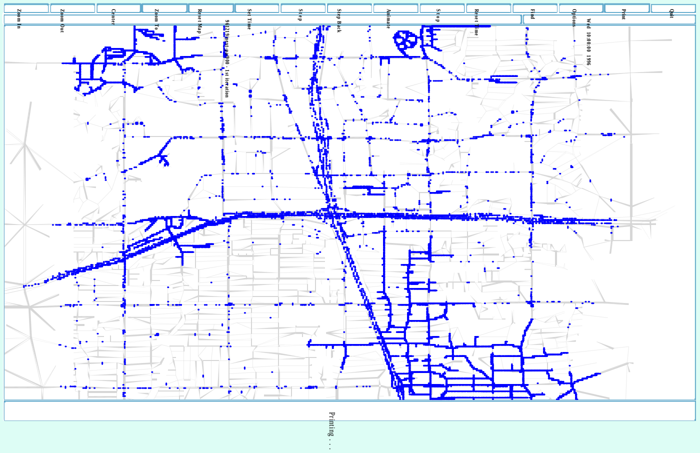
“Spin-up” of an ocean model

Necessary to obtain an internally consistent starting point for solving a coupled system of equations forward in time:

- Velocity = f (Pressure)
- Pressure = g (Salinity, Temperature)
- (Salinity, Temperature) = h(Velocity)

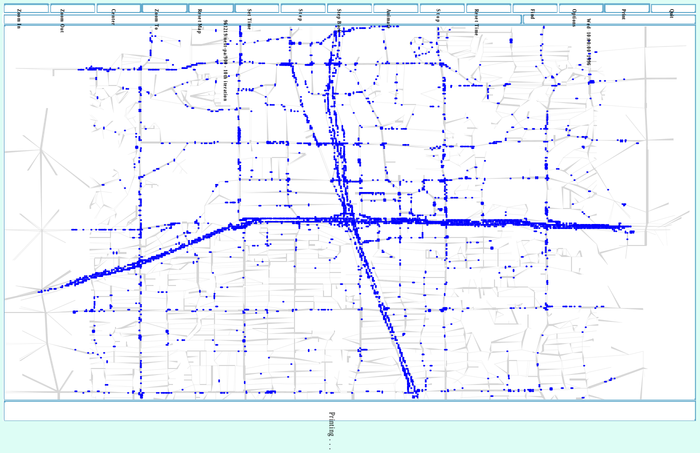
Iteration in TRANSIMS


Iteration 0

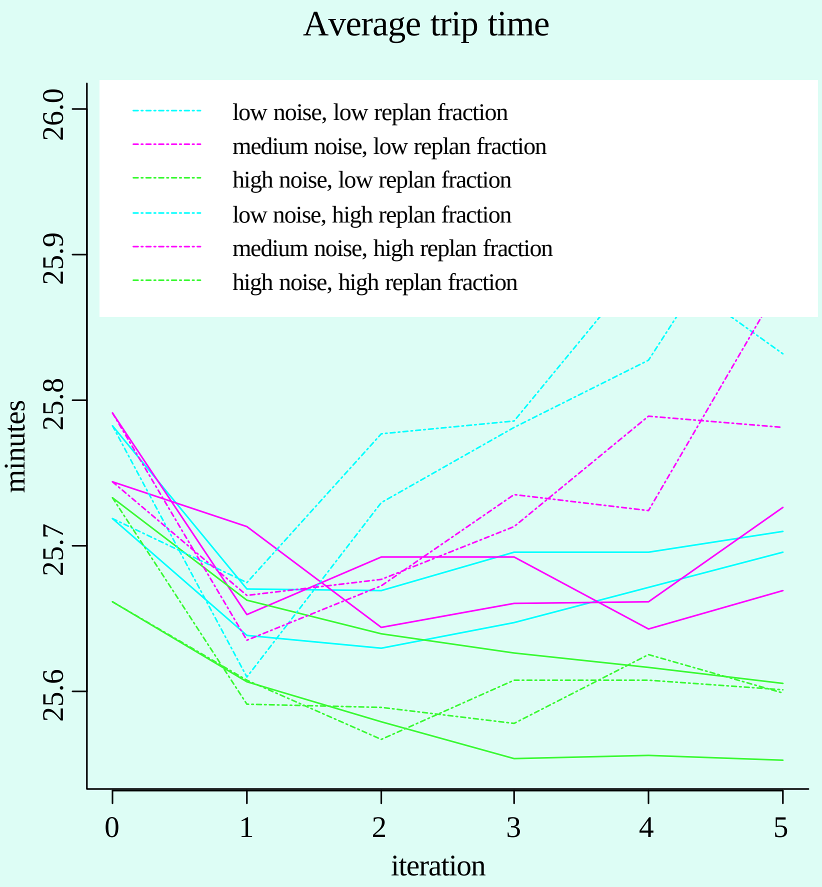

Iteration 1

feedback is required to stabilize a nonlinear system

the iteration process lets activities, route plans, and traffic converge to quasi-equilibrium


Iteration 10

Accelerating Feedback Convergence (Microsimulator to Router)

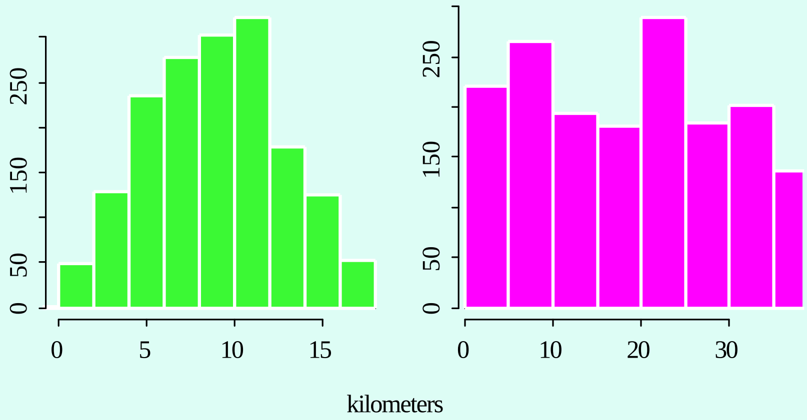


	Iteration			
	0	1	2	3
Replan fraction		0.22	0.17	0.02
Noise level	0.14	0.18	0.00	0.00
Replan × Noise		0.87	0.04	0.09

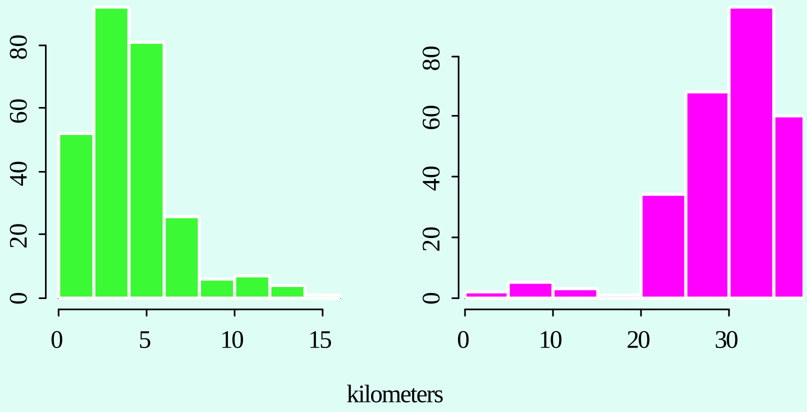
Significance level:
<0.05
<0.10
<0.20

Feedback for Location Assignment (Router to Activity Generator)

Iteration 0 (33.4% of travelers)



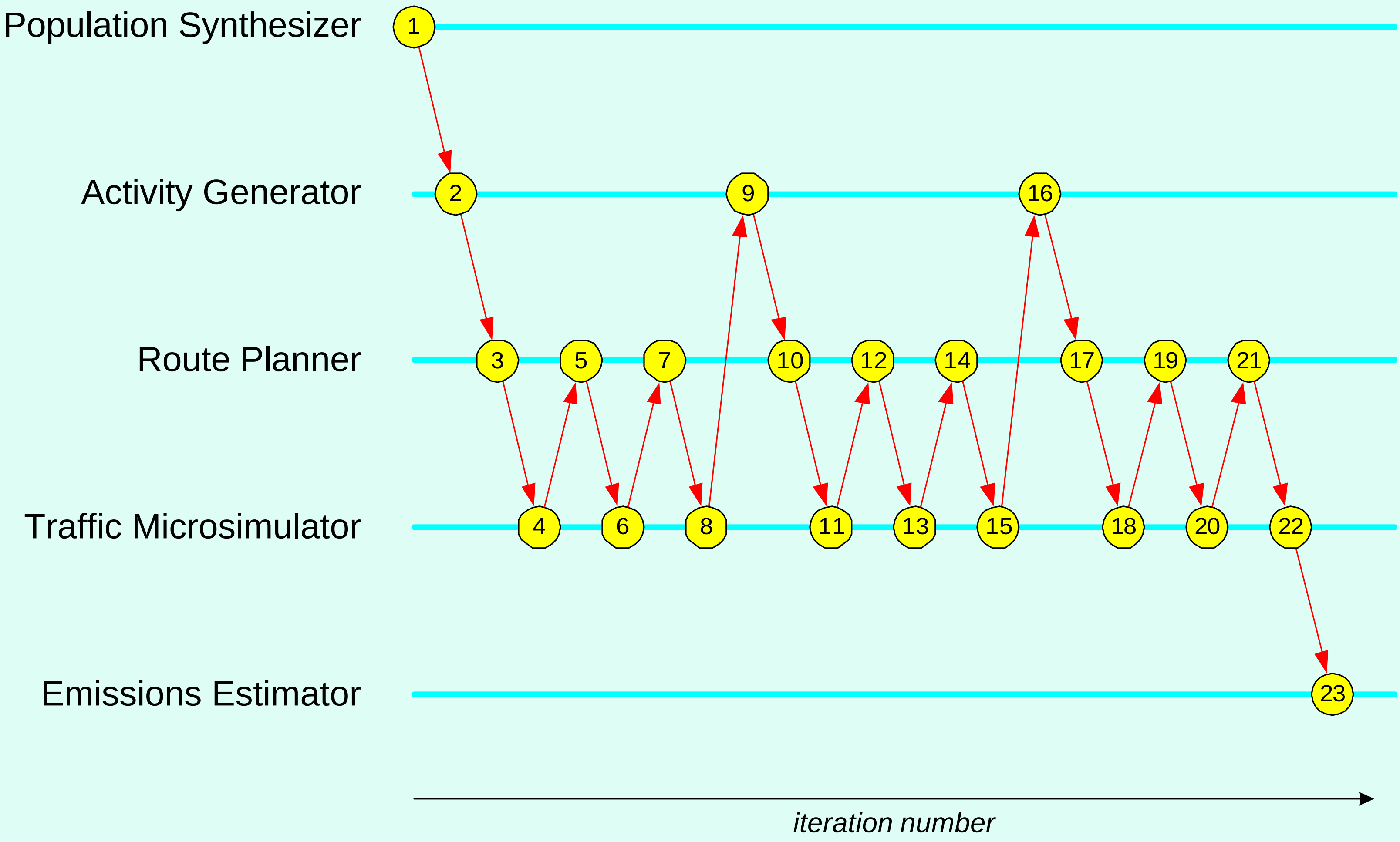
Iteration 10 (5.4% of travelers)



🟩 Access to transit

🟪 Home-to-work distance

Example Study: Strategy for Iterations



Population Synthesizer

Activity Generator

Route Planner

Traffic Microsimulator

Emissions Estimator

iteration number

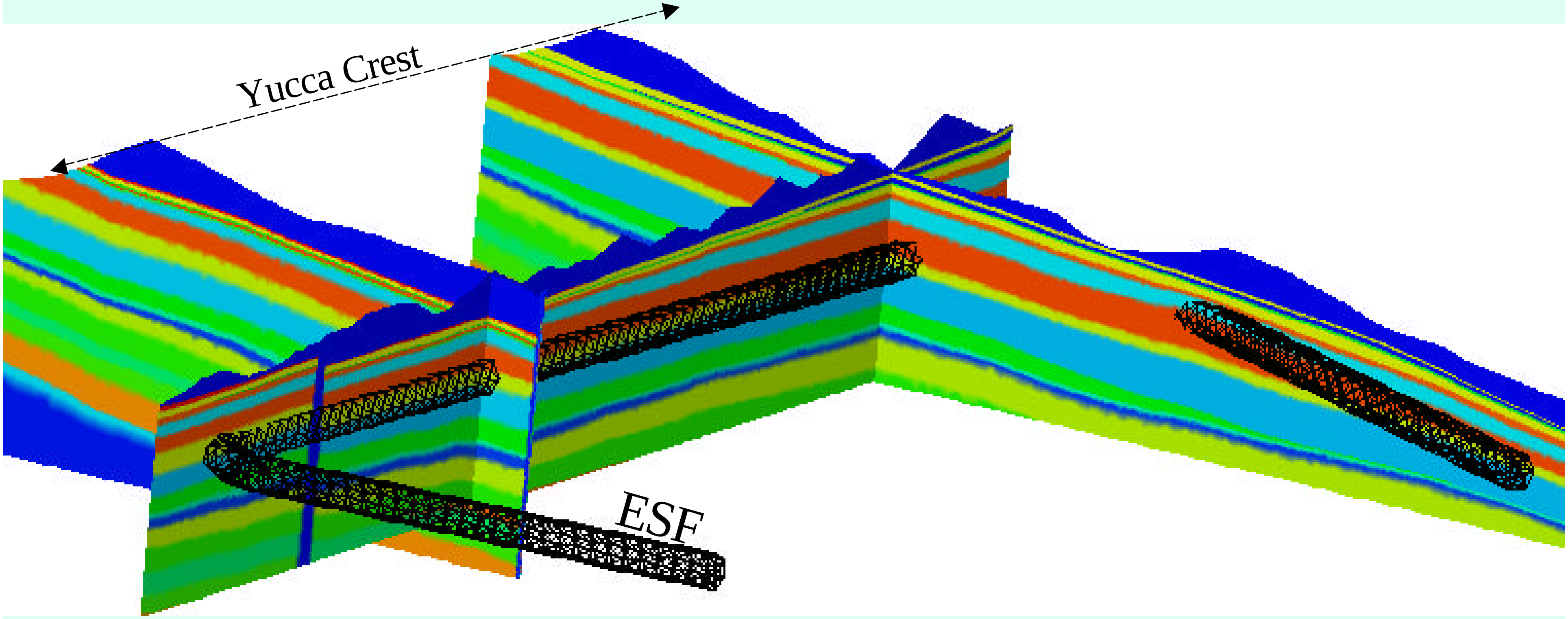
IV. Modeling with TRANSIMS: Model Assessment

- Representation of dynamics
- Boundary conditions
- Calibration
- Assessment
  - Selection and (usually) transformation of available data
  - Generation and (usually) manipulation of computer output
  - Statistical inference

Model assessment questions

- Does the model capture our understanding of the process being modeled?
  - ➢ Does it reproduce some important observable features of this process?
- Does it augment that understanding or provide us with new information?
  - ➢ E.g., what drives the model? the process? And are they the same?
- Can we use it to extrapolate beyond observable conditions?
  - ➢ How much confidence should we attach to model predictions?

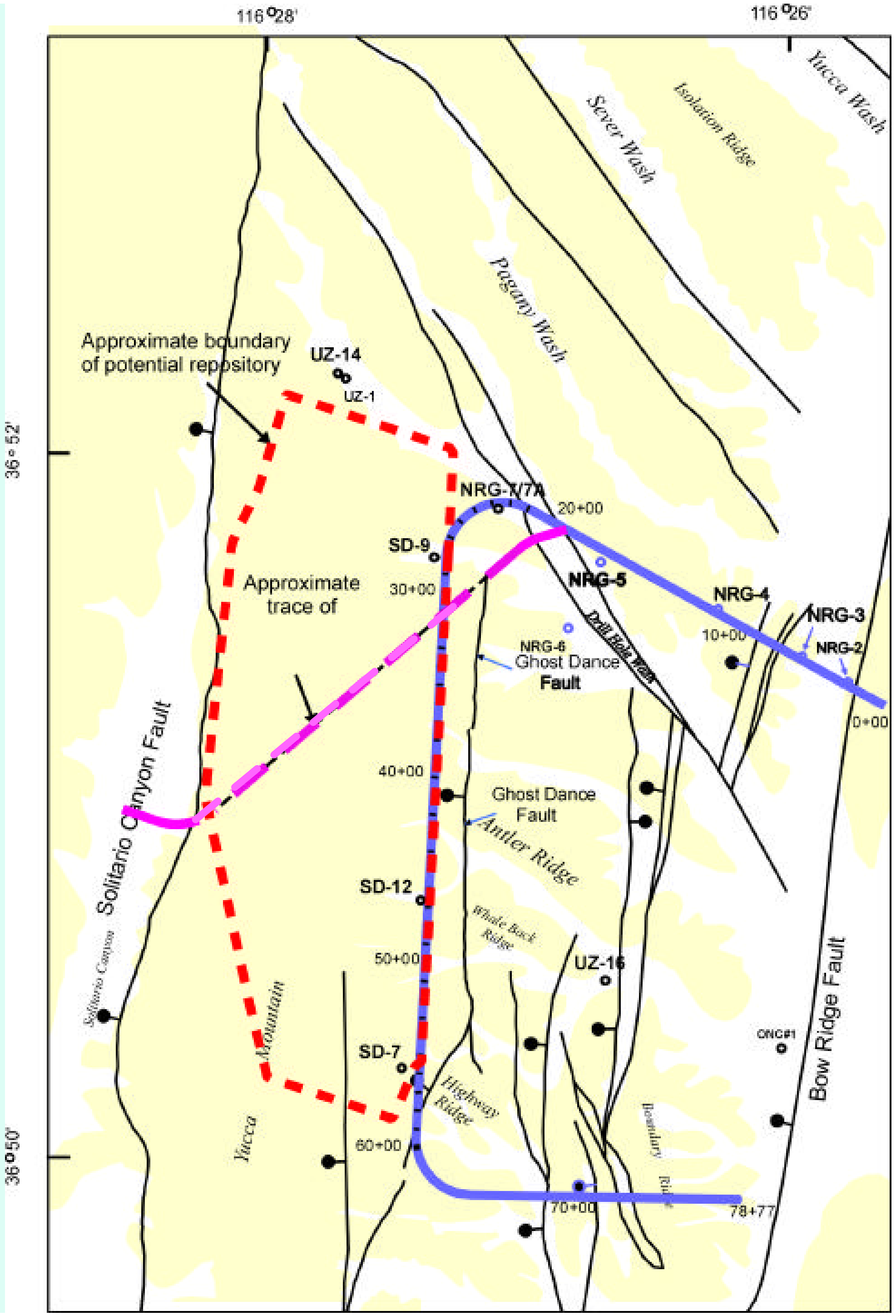
Yucca Mountain Model



Goal: Performance assessment for a potential geologic repository for high-level nuclear wastes

Yucca Mountain Data:

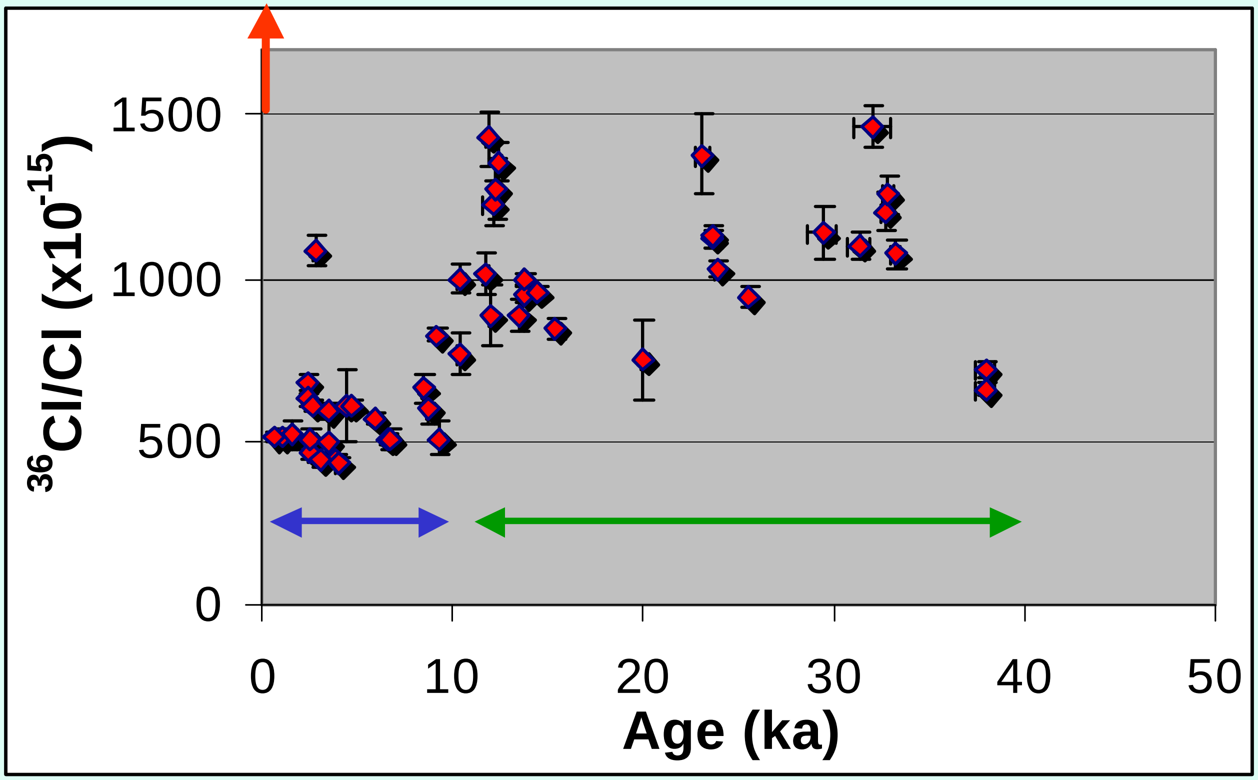
About 200 chlorine-36 samples from the Exploratory Studies Facility, a tunnel (solid blue line) collected at the depth of the potential nuclear waste repository (dashed red line)



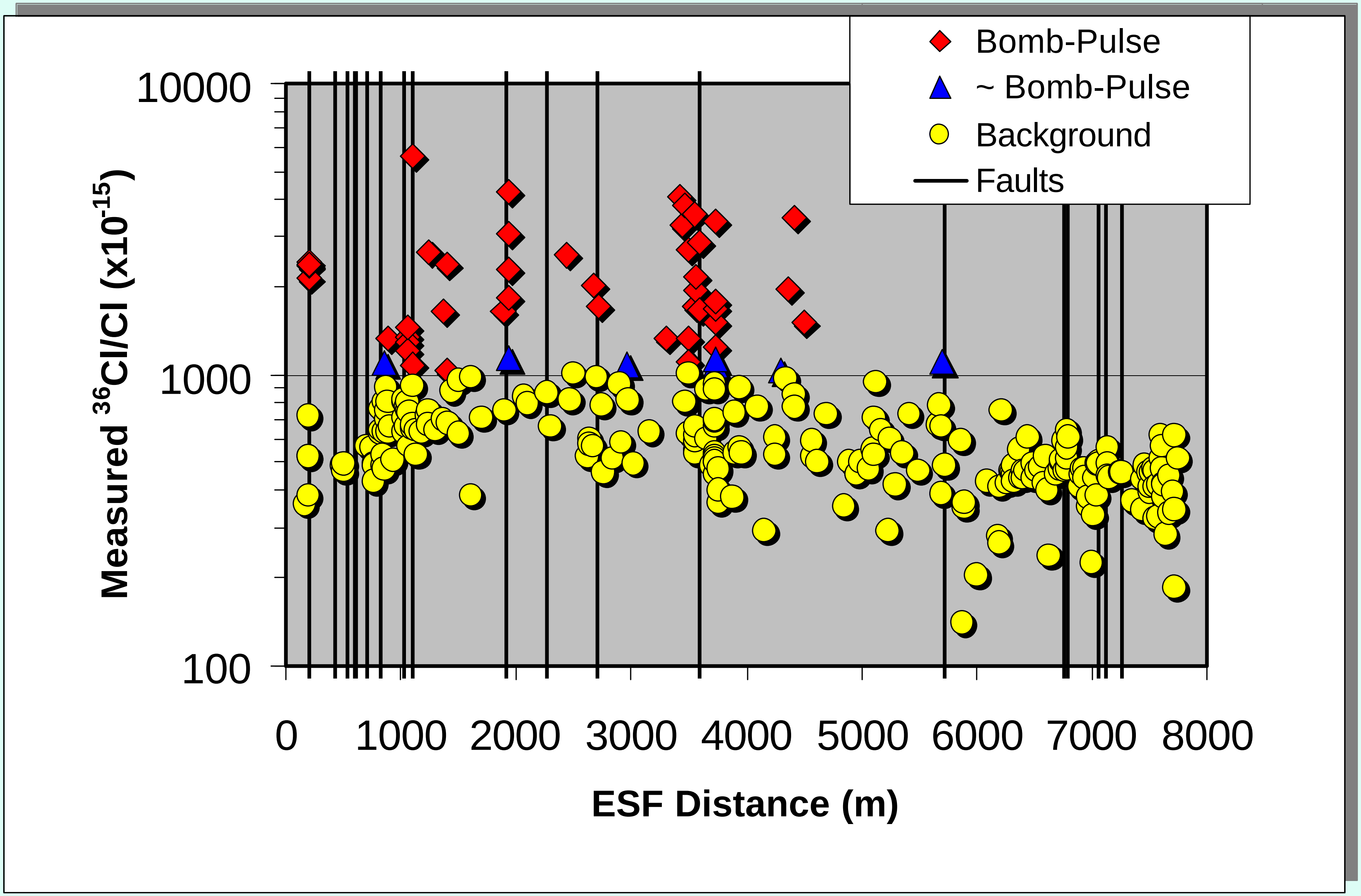
Historic ^{36}Cl/Cl Source Ratio from Plummer et al. (1997)

Three Primary Components:

- Bomb-pulse less than 50 years ago.
- Fairly constant Holocene signal.
- Elevated signal at end of Pleistocene.



Bomb-Pulse Component of Signal



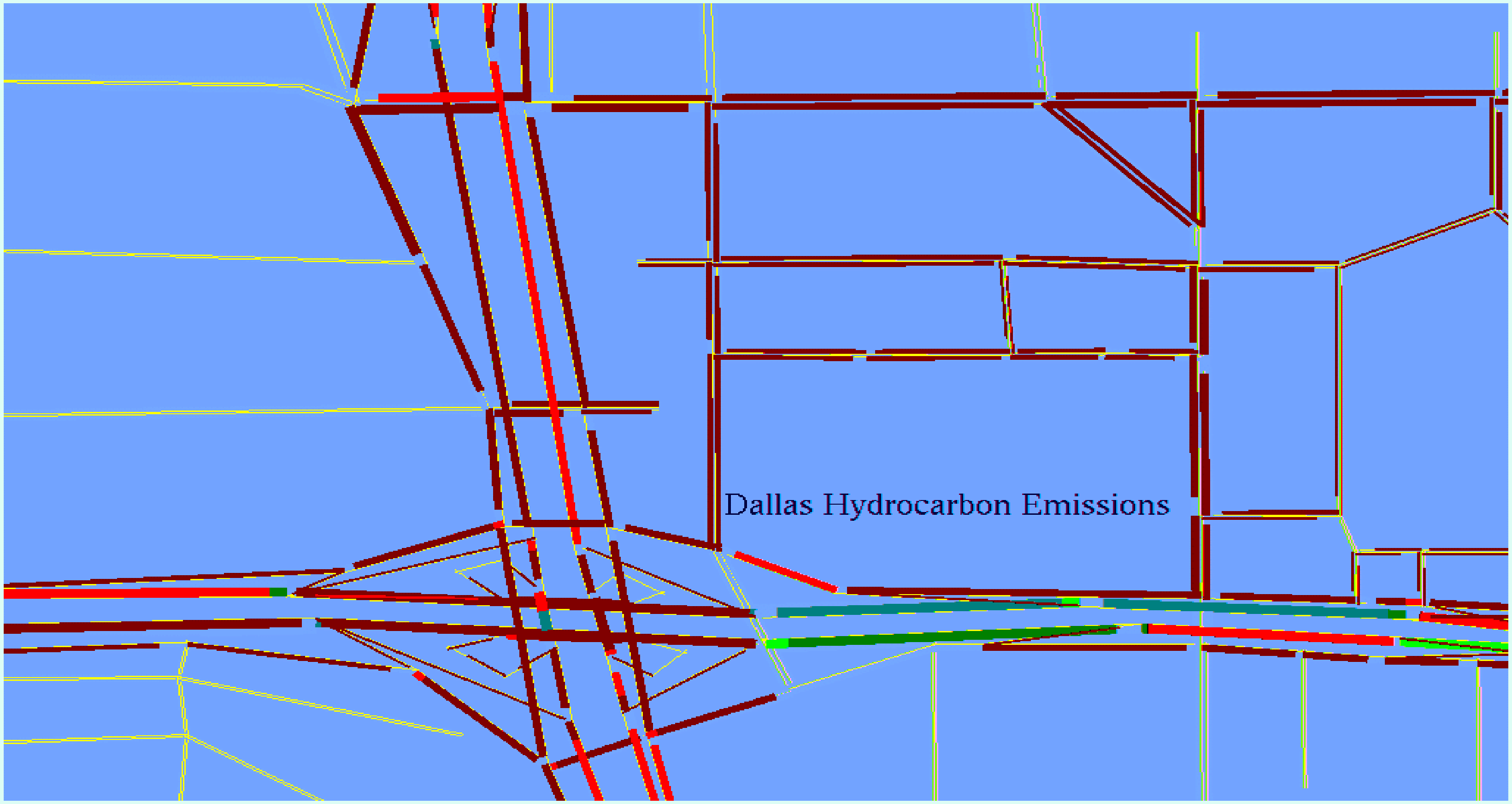
Two explanations for trend

- Above the north end of the tunnel, the PTn retards flow sufficiently that substantial fraction of water is of Pleistocene age
  - Constrains infiltration rates to low end of possible
- Most of the samples in the north end are either below through-cutting faults or in joints that could be connected to such faults by low-angle joints
  - Suggests need for better parameterization of fracture-dominated flow in welded tuff strata

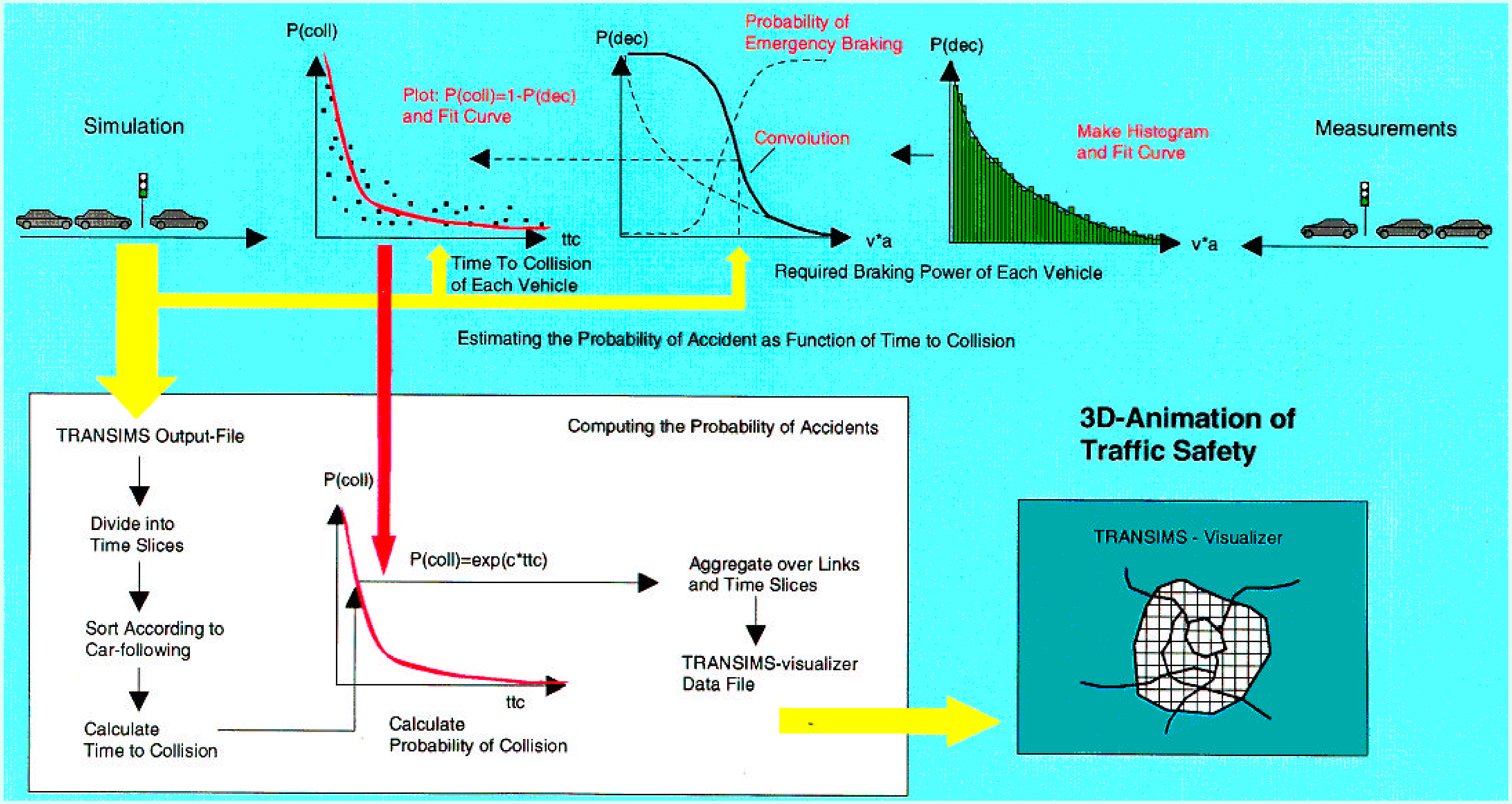
Models and Statistics: Two views into the problem

- Model limitations
  - ➢ Fractures handled by dual permeability/dual porosity type modeling
  - ➢ Heterogeneity within strata is not modeled
- Data limitations
  - ➢ Observations are noisy mixtures of several components
  - ➢ Geology only partially observed (low-angle intersecting joints above tunnel are unobservable)
- Model + Data synergy?

Example Hydrocarbon Emissions in Dallas, Texas



Simulation of Probability of Accidents



Simulation

Plot: P(coll)=1-P(dec) and Fit Curve

Probability of Emergency Braking

Convolution

Make Histogram and Fit Curve

Measurements

Time To Collision of Each Vehicle

Required Braking Power of Each Vehicle

Estimating the Probability of Accident as Function of Time to Collision

Computing the Probability of Accidents

TRANSIMS Output-File

Divide into Time Slices

Sort According to Car-following

Calculate Time to Collision

P(coll)=exp(c*ttc)

Calculate Probability of Collision

Aggregate over Links and Time Slices

TRANSIMS-visualizer Data File

3D-Animation of Traffic Safety

TRANSIMS - Visualizer

V. Conclusions

- Despite the novelty of the TRANSIMS architecture, modeling with TRANSIMS requires the same types of decisions and analyses as modeling with more “traditional” systems.
- Major statistical development is needed, for example,
  - Using models in “inverse” mode to refine (calibrate) input fields (e.g., Kennedy and O’Hagen, Glimm et al., Raftery, …)
  - Standardize to extent possible recommendations and tools for building confidence in models, particularly if they are to be used in decision making or policy contexts.