15 JAHRE
Wissenschaft im Dienst des Menschen

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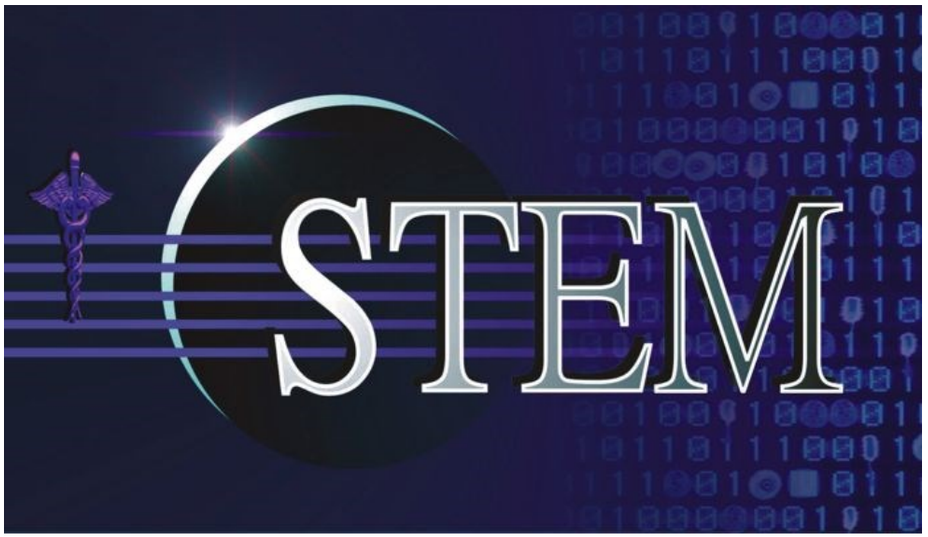
Bundesinstitut für Risikobewertung

BUNDESINSTITUT FÜR RISIKOBEWERTUNG

# STEM - Spatiotemporal Epidemiological Modeler:

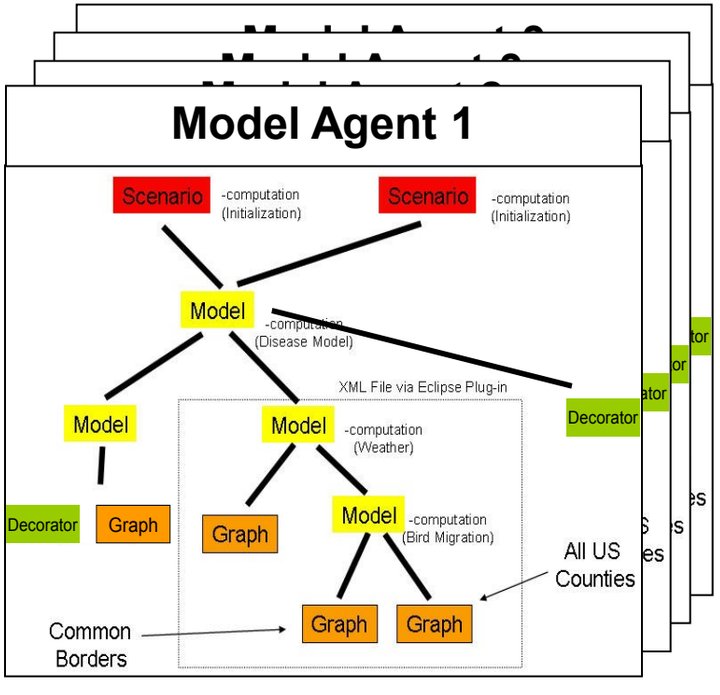
# Overview on Advanced Features

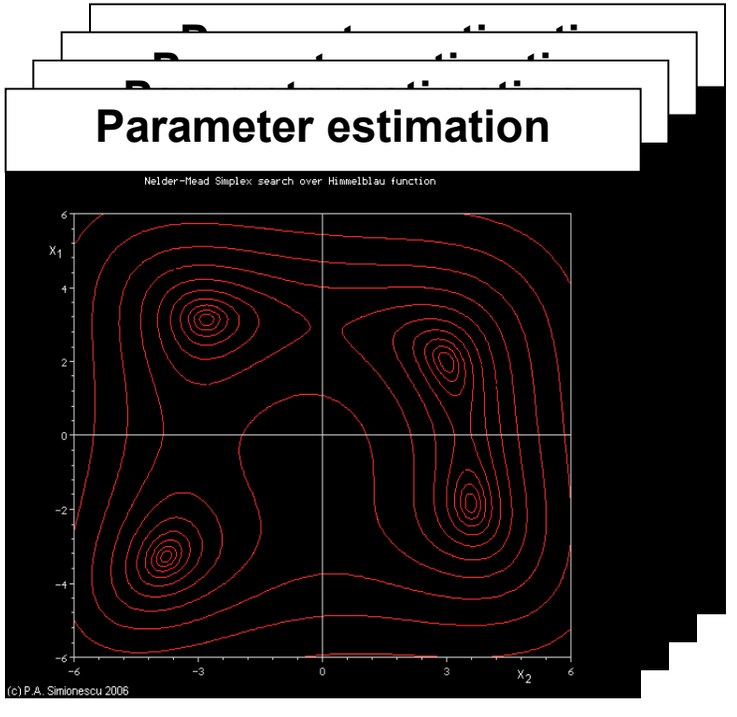



Matthias Filter

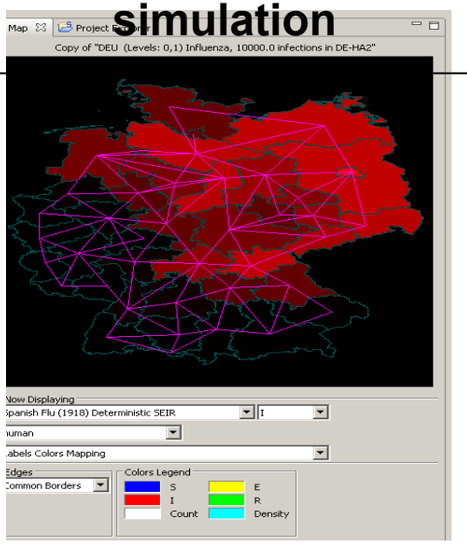
# User Groups

**Knowledge Engineer / Statisticians**



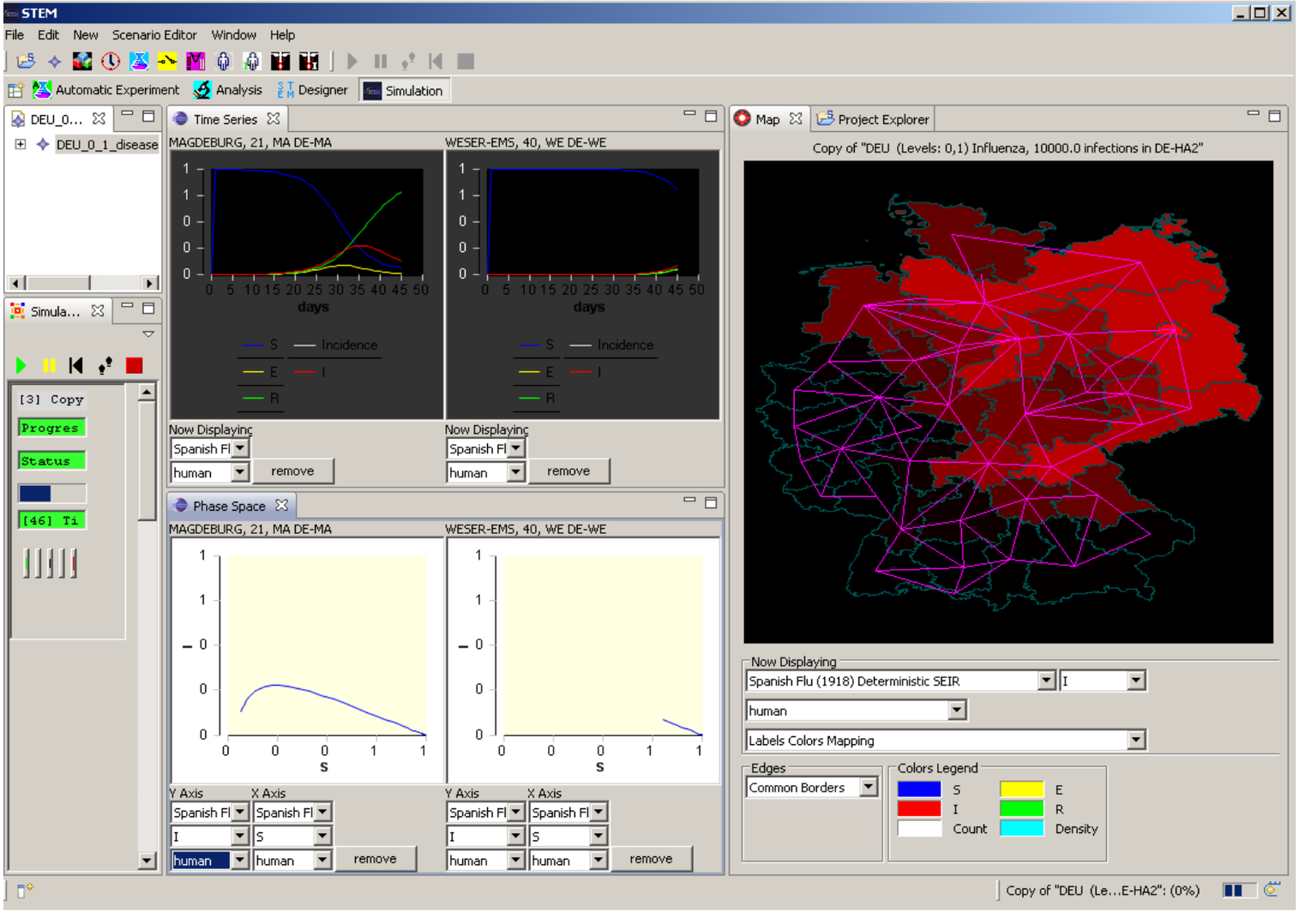




**Library of models for visualization and simulation**




**Public Health Risk Assessor / Manager**

# GUI for simulation, visualization and analysis

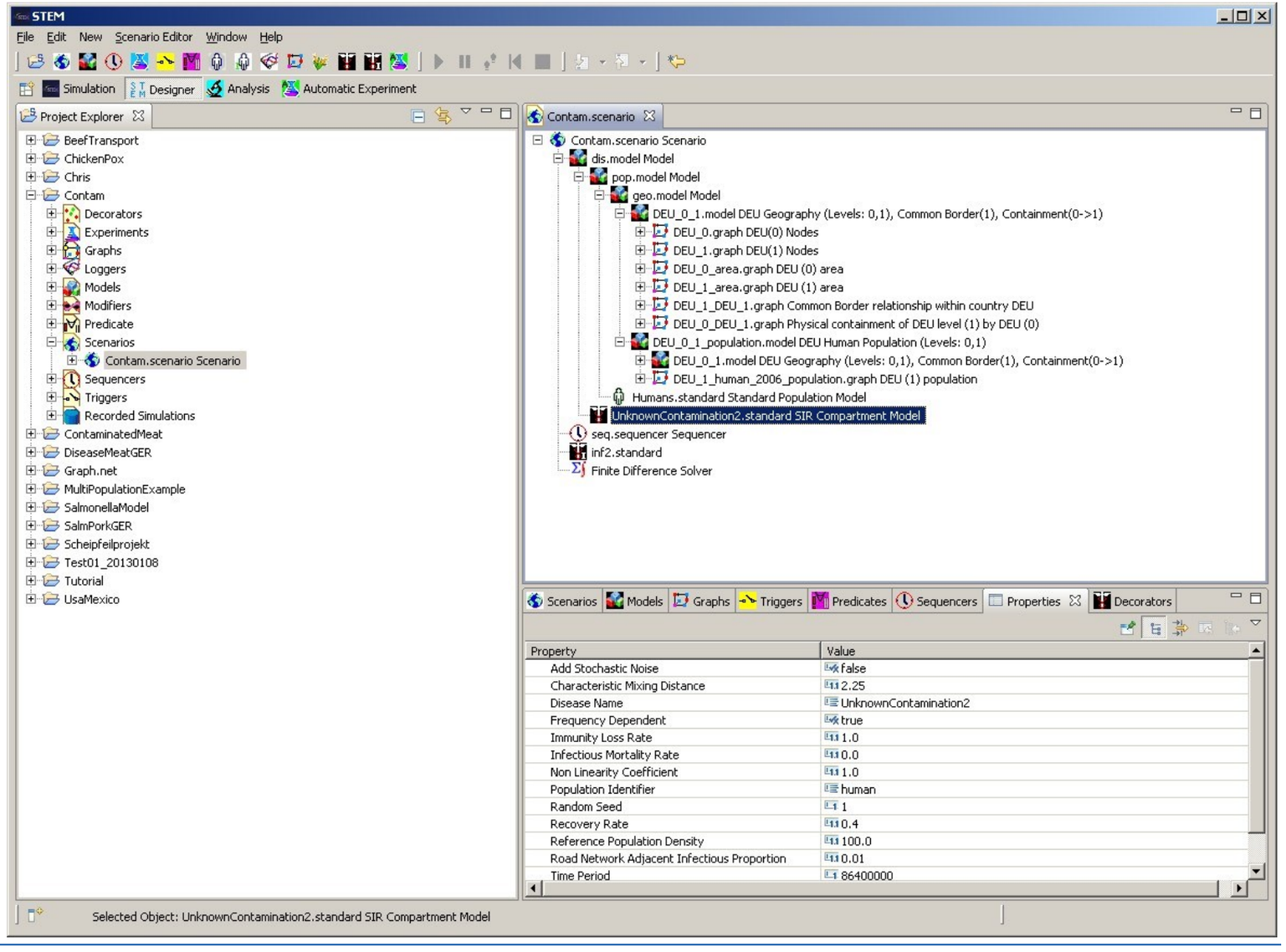


# Integrated Data supporting Global Simulations

Global population data by admin region validated against *LandScan 2007™*

*High Resolution Global Population Data Set*

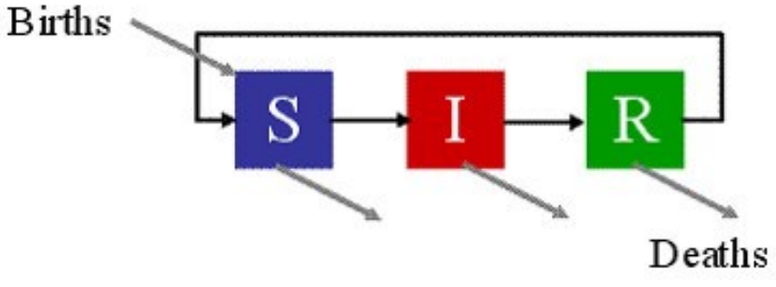
# GUI for scenario and model generation



# Basis I: Epidemiological Models

- Deterministic and stochastic simulations including pre-built compartment models (e.g. SIR, SEIR etc.)
- Code generation tool for new models

## Standard SIR model




Int J Health Geogr. 2006 Jan 17;5:4.
An extensible spatial and temporal epidemiological modelling system.

## Model Equations

$$\Delta S = -\beta (S/P) I + \alpha R + \mu (P-S)$$

$$\Delta I = \beta (S/P) I - \gamma I - \mu I$$

$$\Delta R = \gamma I - \alpha R - \mu R$$

$$\text{Total Population } P = (S + I + R)$$

## Model compartments:

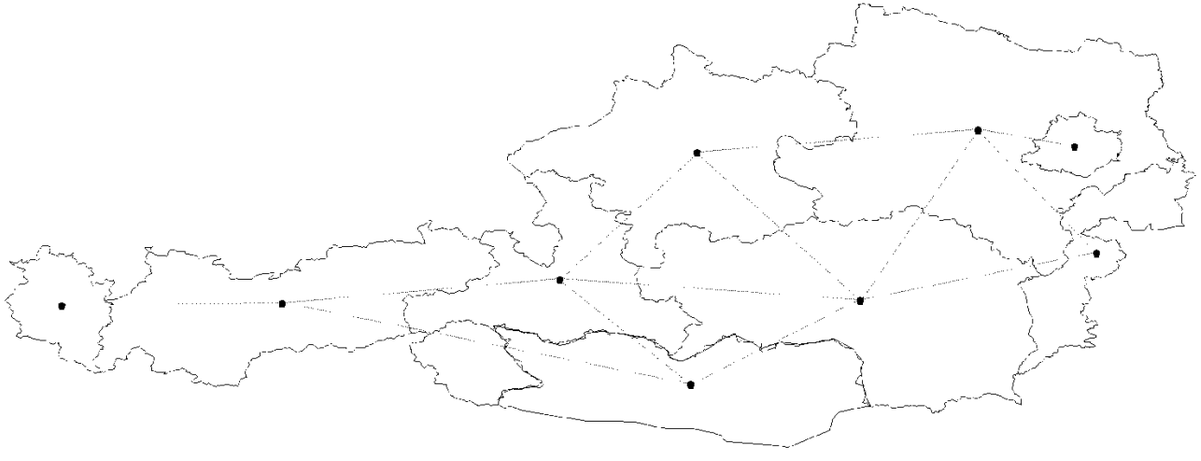
S: Susceptible
I: Infectious
R: Recovered

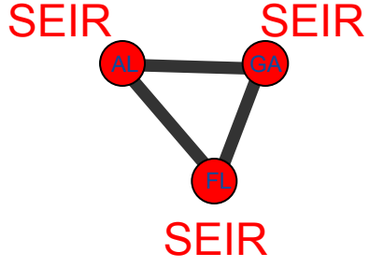
## Model parameters:

- Transmission rate β
- Recovery rate γ
- Immunity loss rate α
- Birth/death rate μ

# Basis II: Spatial distribution of diseases

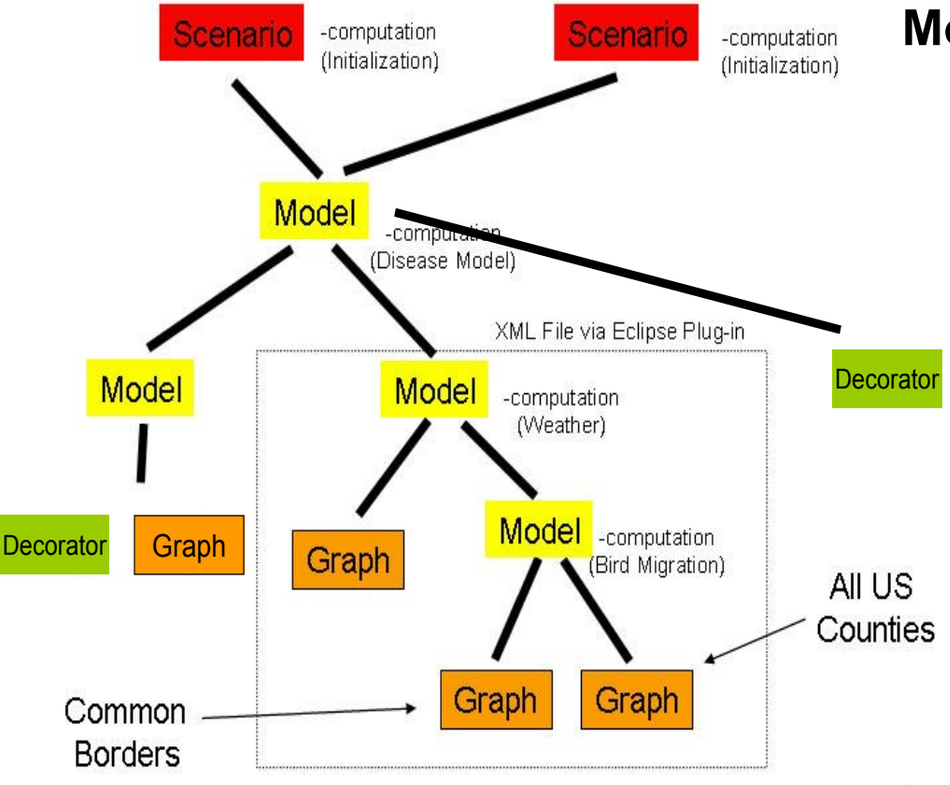
## STEM treats the World as a “Graph”






- Graph = nodes, edges; with labels & decorators
- Graph Framework makes it easy to *build one model on top of another*
- Existing plug-ins define
  - Geography
  - Populations
  - Transportation systems
  - Land area

# Basis III: Canonical Graphs (Integration of all components)




**Scenario**: Model + Infector + Sequencer

**Model**: Graphs + Decorators

**Graphs**: Nodes (Labels) + Edges (Labels) may comprise several subgraphs

Nodes: i.e. places, regions

Edges: i.e. relationships, connections between nodes, vectors

**Decorators**: denominator data and model parameters

Disease: Disease model parameter

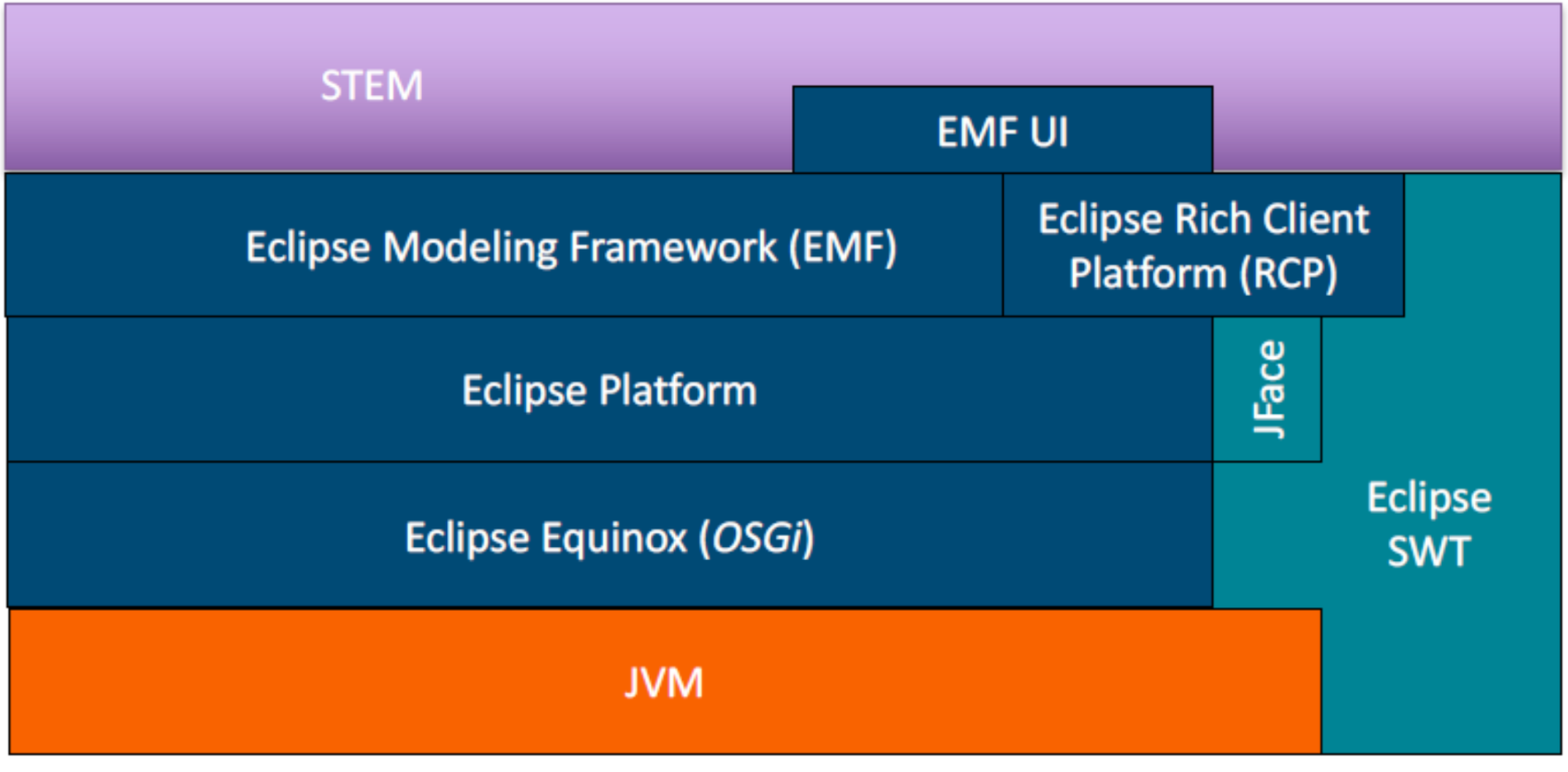
Modifier: Parameter tuning components

**Infector**: Disease initiation parameters

**Sequencer**: Simulation time parameter

# Basis IV: STEM Software Architecture (and language)

- Built on Eclipse Platform and Modeling Framework, SWT/JFace/RCP UI



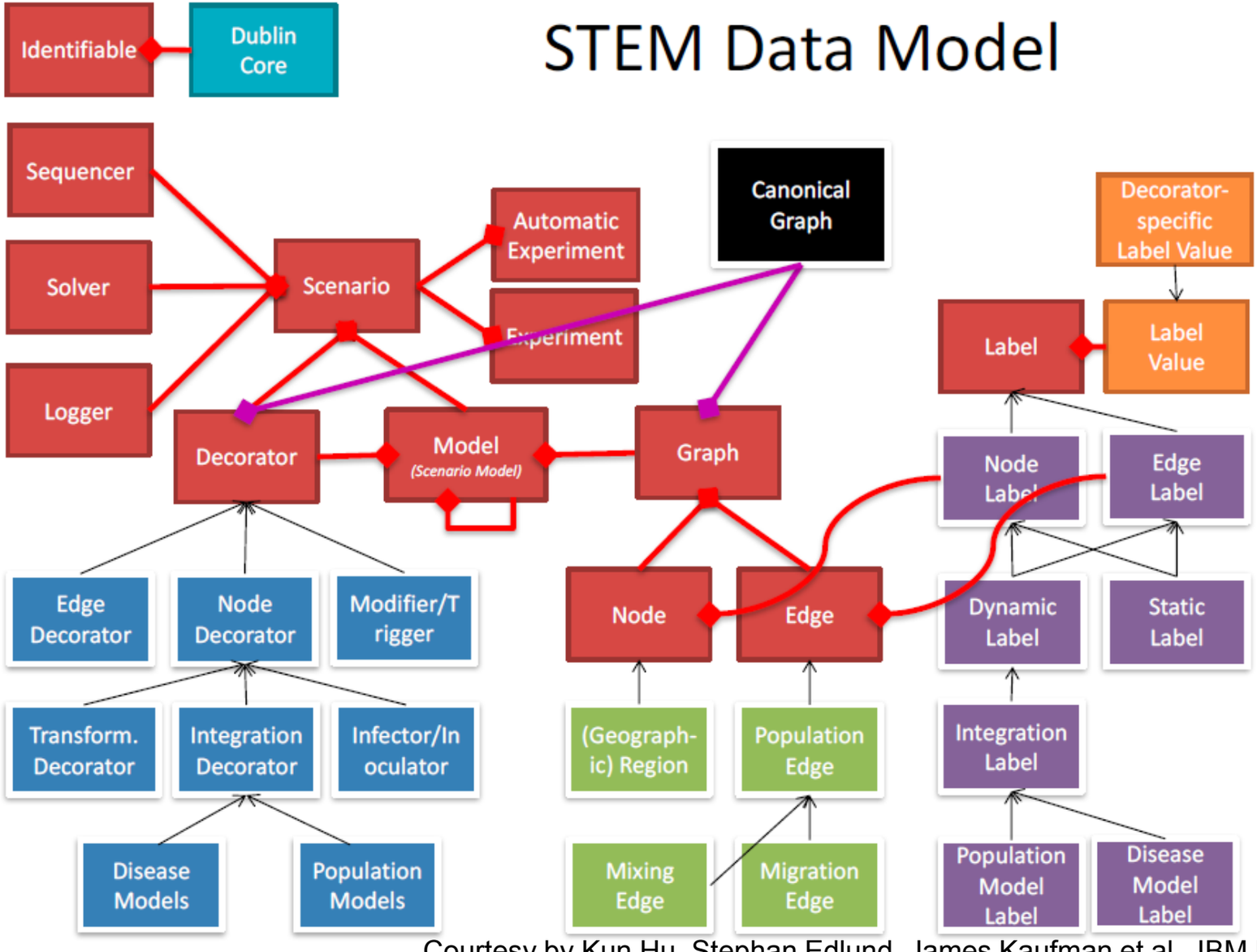

Courtesy by Kun Hu, Stephan Edlund, James Kaufman et al., IBM Research,

# STEM Terminology ("What is meant by "Model")

- We use the word "Model" interchangeably
- Depending upon context, it'll be related to one of the following:
  - Data modeled, code-generated data structures (**STEM Data Model or EMF Models**)
  - Container in STEM UI for composing scenarios (**Scenario Model or Geographic model**)
  - Dynamic, integrated, programmatic models (**Disease or population model**, like Influenza)
  - **Model builder** – tool for authoring disease models

Courtesy by Kun Hu, Stephan Edlund, James Kaufman et al., IBM Research,

# Basis V: STEM Data Model




Courtesy by Kun Hu, Stephan Edlund, James Kaufman et al., IBM Research,

# STEM Components

- Core
  - Core data (EMF) models
    - Identifiable, Scenario, Model, Graph (Node/Edge), Decorators, Labels, …
  - Simulation Engine (org.eclipse.stem.jobs)
  - Solver, sequencer, logger, graph generator implementations
- Data
  - Geography, Population, Transportation, Earth Science
  - Tools for generating fixed plug-ins of data components (“built-in data”)
- Epidemiological models
  - Disease Model implementations (SI, SIR, SEIR, Multi-population, Malaria, Polio, etc)
  - Sample diseases
- Population models
  - Dynamic population models (e.g. mosquito population)
- Food Production models
- Model Generator
- User Interface for all of the above

Courtesy by Kun Hu, Stephan Edlund, James Kaufman et al., IBM Research,

# STEM Canonical Graph

- The runtime representation of a simulation's state
  - *simulation.getScenario().getCanonicalGraph()*
- Generated from the Scenario when a simulation is started
  - Flattened and resolved version of the combined Graphs supplied to the Scenario
- Contains
  - Decorators
  - Nodes
  - Edges
  - Time

Courtesy by Kun Hu, Stephan Edlund, James Kaufman et al., IBM Research,

# STEM Decorators

- Objects that act on the canonical graph by **creating** and **updating** Labels
  - Decorators “decorate” the graph
- Can act on the graph, nodes, or edges
  - Applied to the (geographic) model or scenario
- Decorator examples
  - Disease models (Integration Decorator)
  - Dynamic population models
  - Infectors, innoculators
  - Triggers, modifiers

Courtesy by Kun Hu, Stephan Edlund, James Kaufman et al., IBM Research,

# STEM Labels

- Objects containing simulation state data attached to nodes and edges
- Both static (fixed values) and dynamic (variable values)
  - Integration labels provide for numerical integration of current and next values
- Labels contain one or more **LabelValue** objects with the label's property values

Courtesy by Kun Hu, Stephan Edlund, James Kaufman et al., IBM Research,

# STEM Labels Examples

## Static Labels

- Node Labels
  - Census human population
  - Area
  - Elevation
  - Earth Science
    - Temperature, nighttemp, relative humidity
- Edge labels
  - Physical Relationships
    - Common Border
    - Physical Containment
  - Migration rate between nodes
  - Transportation rate

## Dynamic Labels

- Dynamic Node Labels
  - Disease model compartment states
  - Dynamic population models
    - E.g. vector-borne

Courtesy by Kun Hu, Stephan Edlund, James Kaufman et al., IBM Research,

# STEM Labels – How they work

- A disease model provides a **Label** and **LabelValue**
- A STEM simulation contains
  - A single instance of the disease model (Decorator)
  - A label for each region in geographic model
- A disease model's label contains *current* and *next* **LabelValue** objects that store the compartment states for the node
  - Example: A SIR disease model's LabelValues contains s, i, and r properties
- The Solver calls *calculateDeltas(…)* on the Decorator, which is responsible for calculating the Label's `nextValue`
- The solver integrates between the values

Courtesy by Kun Hu, Stephan Edlund, James Kaufman et al., IBM Research,

# STEM: Advanced Features

- Advanced Population Initialization (Structured Populations, Aging Populations)

- Advanced Disease Initialization (Infectors, Inoculators, and Initializers)

- Working with Graphs
  - Composing a Graph
  - Creating a Custom Graph
  - Visualizing and Editing Graphs with the STEM Graph Editor
  - Importing a Graph from a Pajek File
  - Importing a Graph from an Esri Shapefile
  - Import Discrete Transportation Events

- Triggering Interventions
- Running Experiments (in batch mode)
- Invoking Modifiers Using Triggers and Predicates.

# STEM: Advanced Features

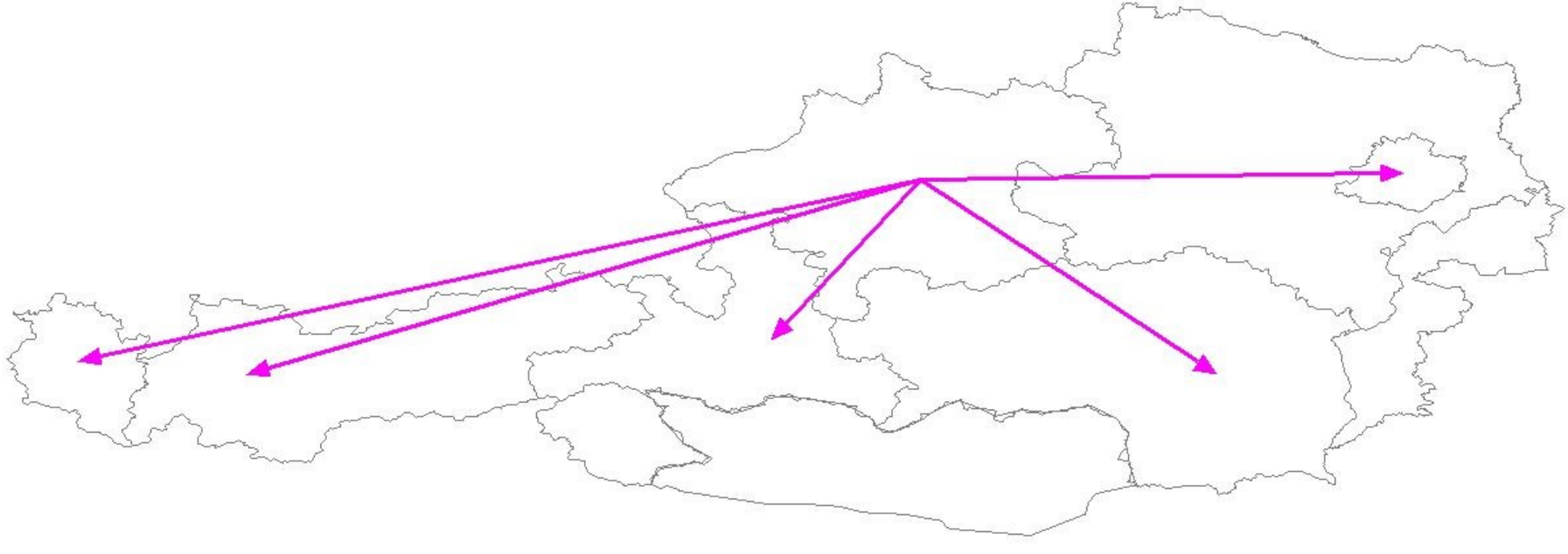
- Logging Data to Files / Importing Data from Files
- STEM Model Creator
- Running an Automated Experiment / STEM Analysis Perspective
  - Estimating Model Parameters from External Data
  - Epidemic Analysis
  - RMS Comparison Between Data Sets
  - Lyapunov Analysis
- Running STEM Headless
- Etc.

# Working with Graphs
# Pajek Net Graph Generator

Pajek-like format

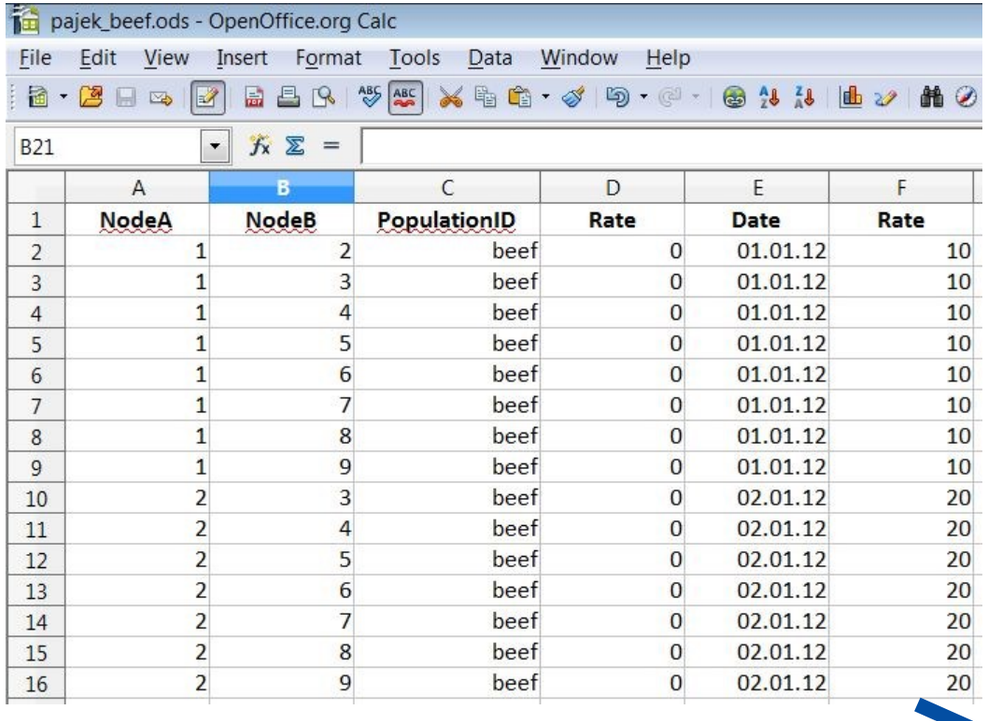
Define movement (disease vectors, travel, transportation events,)

```
*Vertices 9
1 AT-10
2 AT-2
3 AT-3
4 AT-4
5 AT-5
6 AT-6
7 AT-7
8 AT-8
9 AT-9
*Edges
1 2 popID beef rate 0 date 01.01.12 rate 10
1 3 popID beef rate 0 date 01.01.12 rate 10
1 4 popID beef rate 0 date 01.01.12 rate 10
1 5 popID beef rate 0 date 01.01.12 rate 10
1 6 popID beef rate 0 date 01.01.12 rate 10
```



# Pajek Net Graph Generator

## Open Office Macro



pajek_beef.ods - OpenOffice.org Calc

File Edit View Insert Format Tools Data Window Help

B21

| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| 1 | NodeA | NodeB | PopulationID | Rate | Date | Rate |
| 2 | 1 | 2 | beef | 0 | 01.01.12 | 10 |
| 3 | 1 | 3 | beef | 0 | 01.01.12 | 10 |
| 4 | 1 | 4 | beef | 0 | 01.01.12 | 10 |
| 5 | 1 | 5 | beef | 0 | 01.01.12 | 10 |
| 6 | 1 | 6 | beef | 0 | 01.01.12 | 10 |
| 7 | 1 | 7 | beef | 0 | 01.01.12 | 10 |
| 8 | 1 | 8 | beef | 0 | 01.01.12 | 10 |
| 9 | 1 | 9 | beef | 0 | 01.01.12 | 10 |
| 10 | 2 | 3 | beef | 0 | 02.01.12 | 20 |
| 11 | 2 | 4 | beef | 0 | 02.01.12 | 20 |
| 12 | 2 | 5 | beef | 0 | 02.01.12 | 20 |
| 13 | 2 | 6 | beef | 0 | 02.01.12 | 20 |
| 14 | 2 | 7 | beef | 0 | 02.01.12 | 20 |
| 15 | 2 | 8 | beef | 0 | 02.01.12 | 20 |
| 16 | 2 | 9 | beef | 0 | 02.01.12 | 20 |

```
*Vertices 9
1 AT-10
2 AT-2
3 AT-3
4 AT-4
5 AT-5
6 AT-6
7 AT-7
8 AT-8
9 AT-9
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1 2 popID beef rate 0 date 01.01.12 rate 10
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1 5 popID beef rate 0 date 01.01.12 rate 10
1 6 popID beef rate 0 date 01.01.12 rate 10
1 7 popID beef rate 0 date 01.01.12 rate 10
1 8 popID beef rate 0 date 01.01.12 rate 10
1 9 popID beef rate 0 date 01.01.12 rate 10
2 3 popID beef rate 0 date 02.01.12 rate 20
2 4 popID beef rate 0 date 02.01.12 rate 20
2 5 popID beef rate 0 date 02.01.12 rate 20
2 6 popID beef rate 0 date 02.01.12 rate 20
2 7 popID beef rate 0 date 02.01.12 rate 20
2 8 popID beef rate 0 date 02.01.12 rate 20
2 9 popID beef rate 0 date 02.01.12 rate 20
```
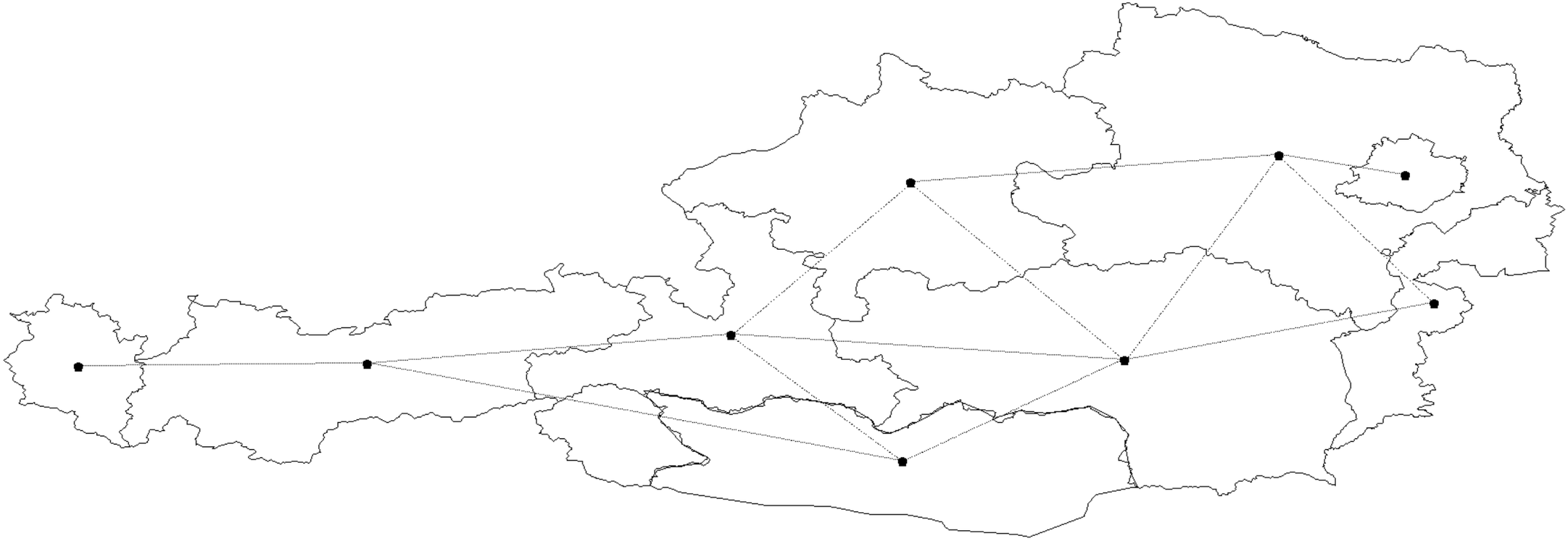
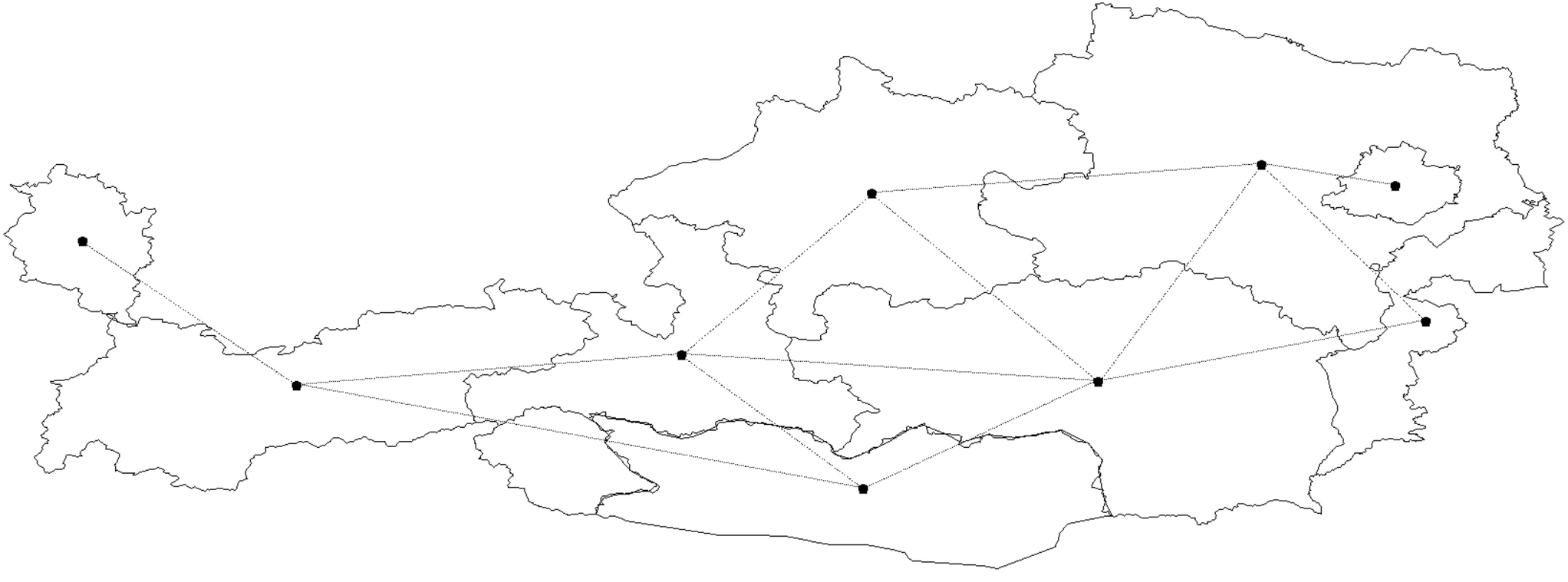
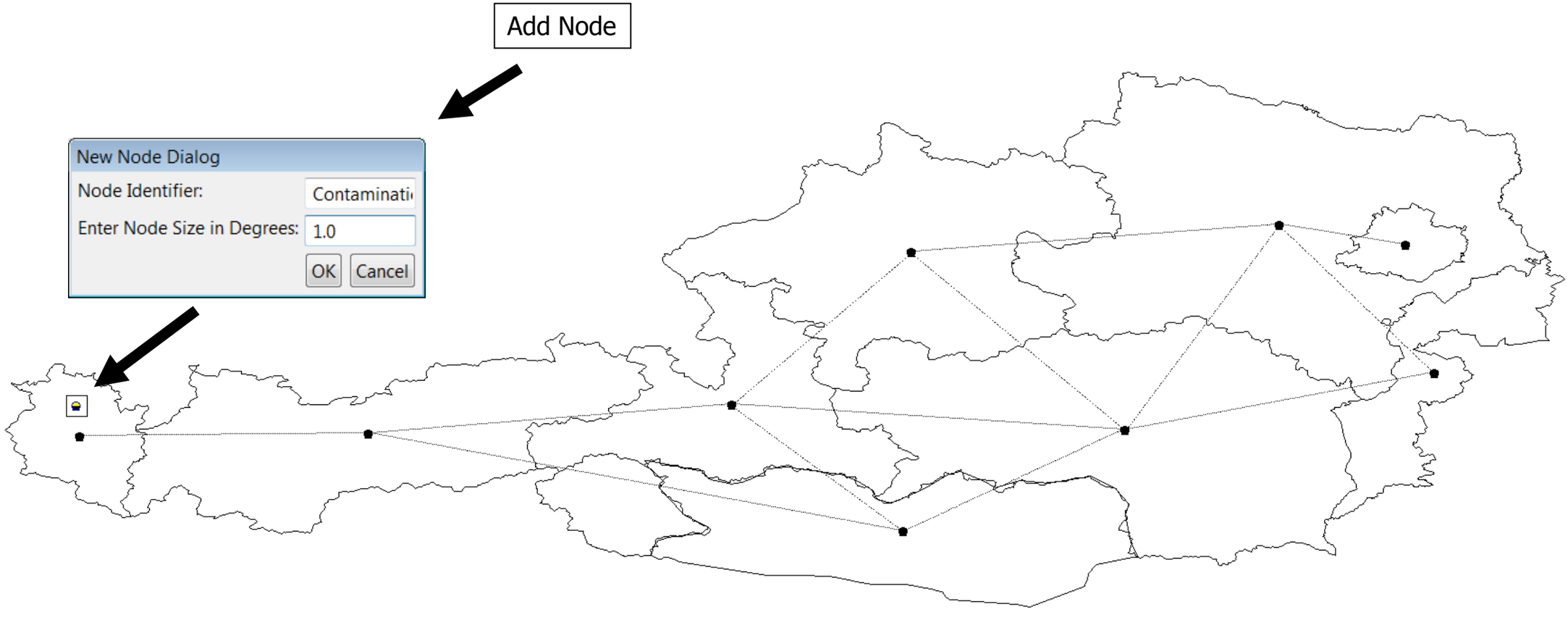

# Graph Editor



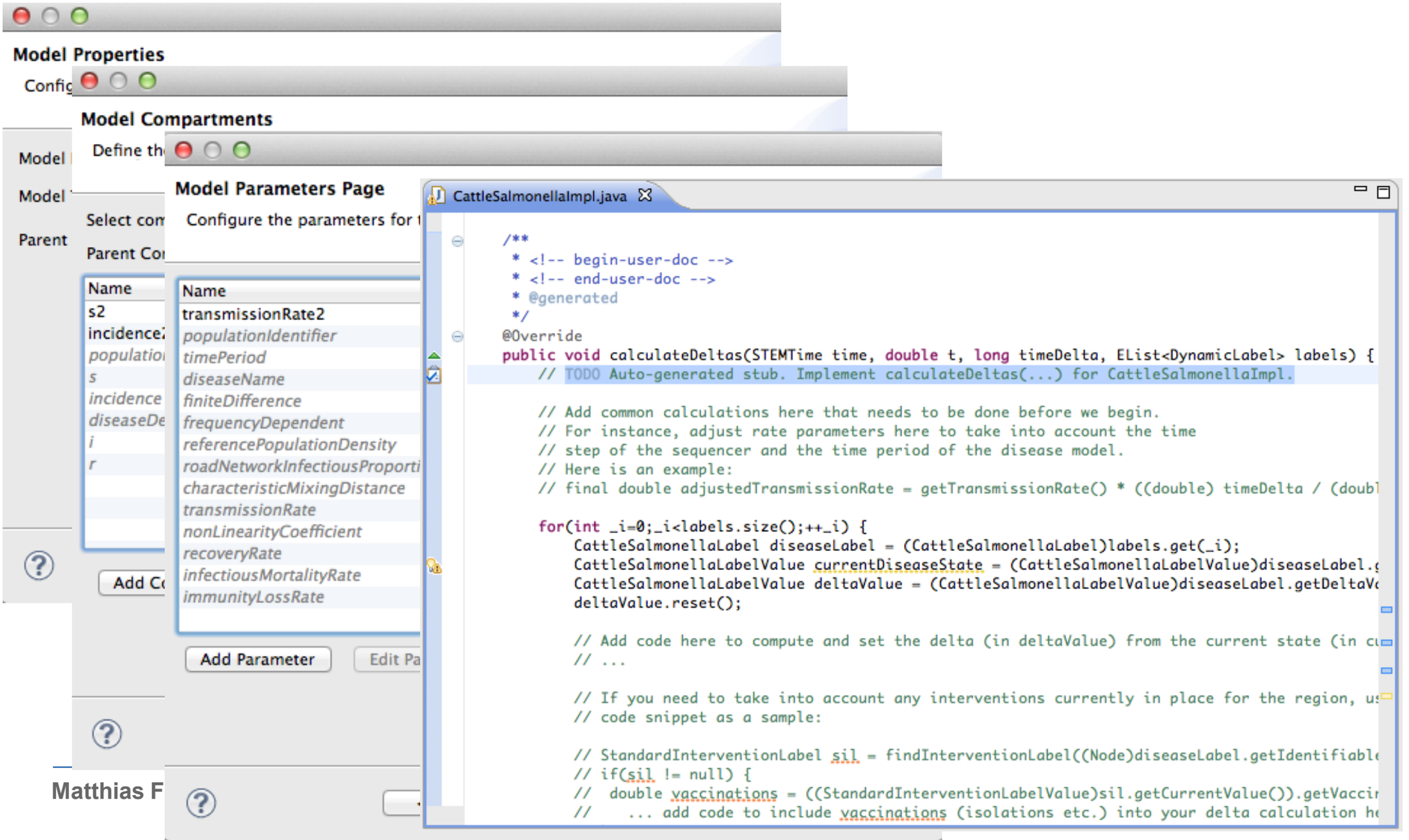
# Graph Editor



# Graph Editor

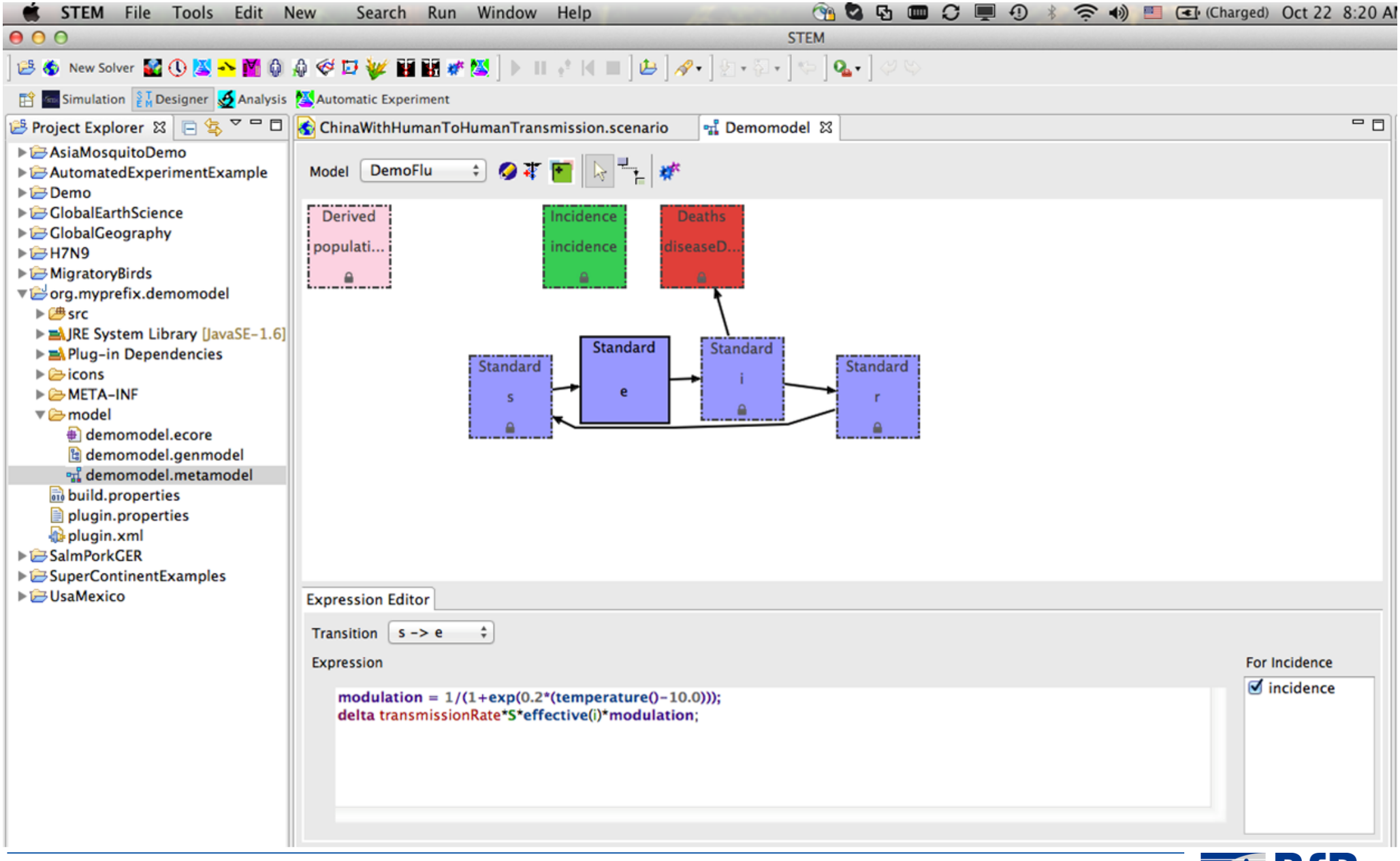


# STEM Model Creator




Matthias F

# STEM Visual Editor



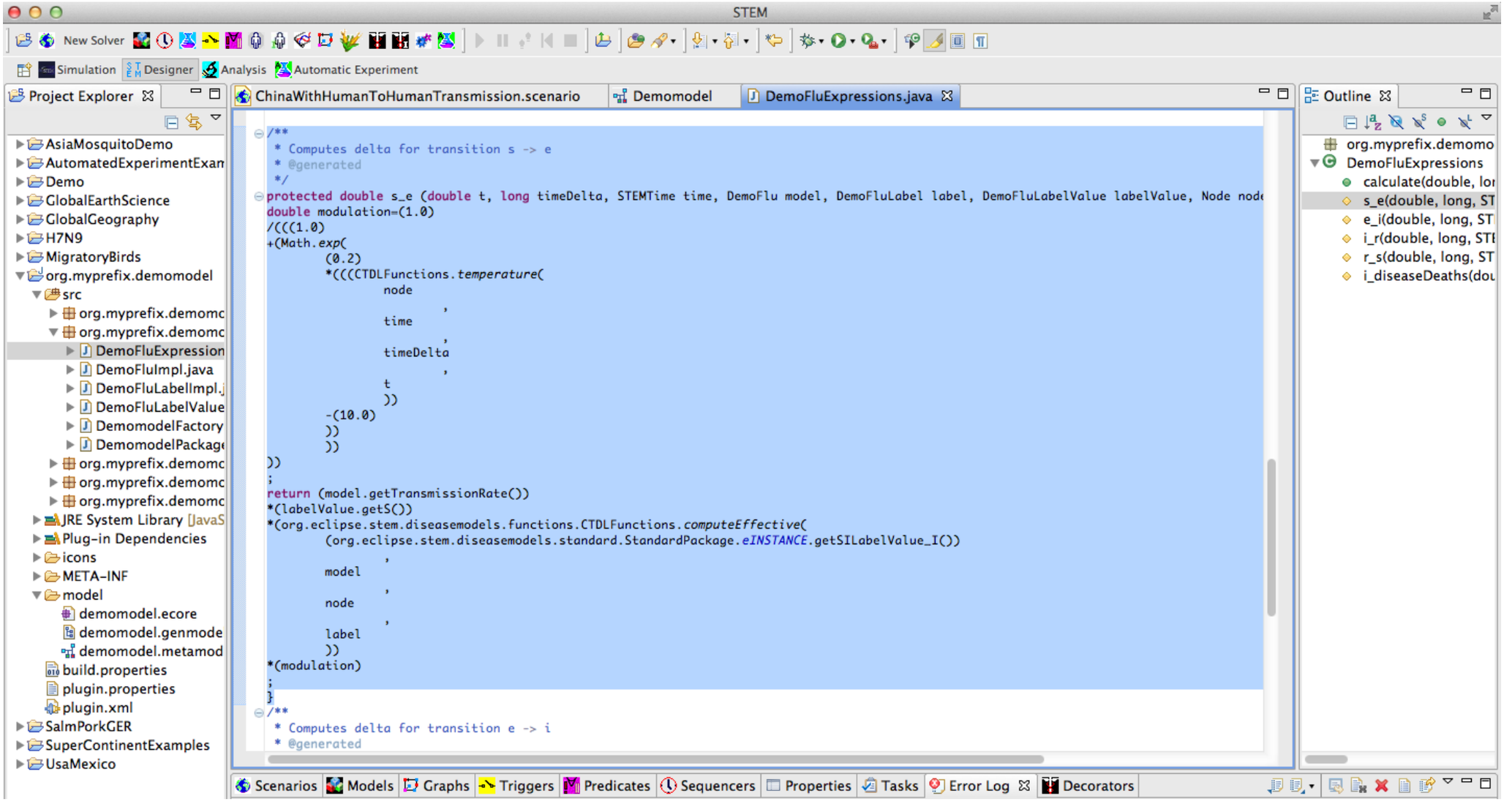
# Expression Language


- Domain-specific grammar for scientists
- Used to define transition rates between compartments
- “Hide the complexity” of STEM’s graph and data APIs
  - Bridge gap between literature and technology
- “Just-In-Time”: Interpret, compile, and inject “hot” code into running JVM
  - Integrates with Metamodel, Code Generator

# STEM Visual Editor


- Visual Editor connects Model Generator and Expression Language in usable way
- Powered by Eclipse Graphical Editing Framework (GEF)
- Diagram Editor: adding, editing, removing compartments and transitions
- Expression Editor: specify conditions in Expression language
  - Code assistance
  - User documentation with NLS (Eclipse Babel)

# Generated Code is Fully Transparent

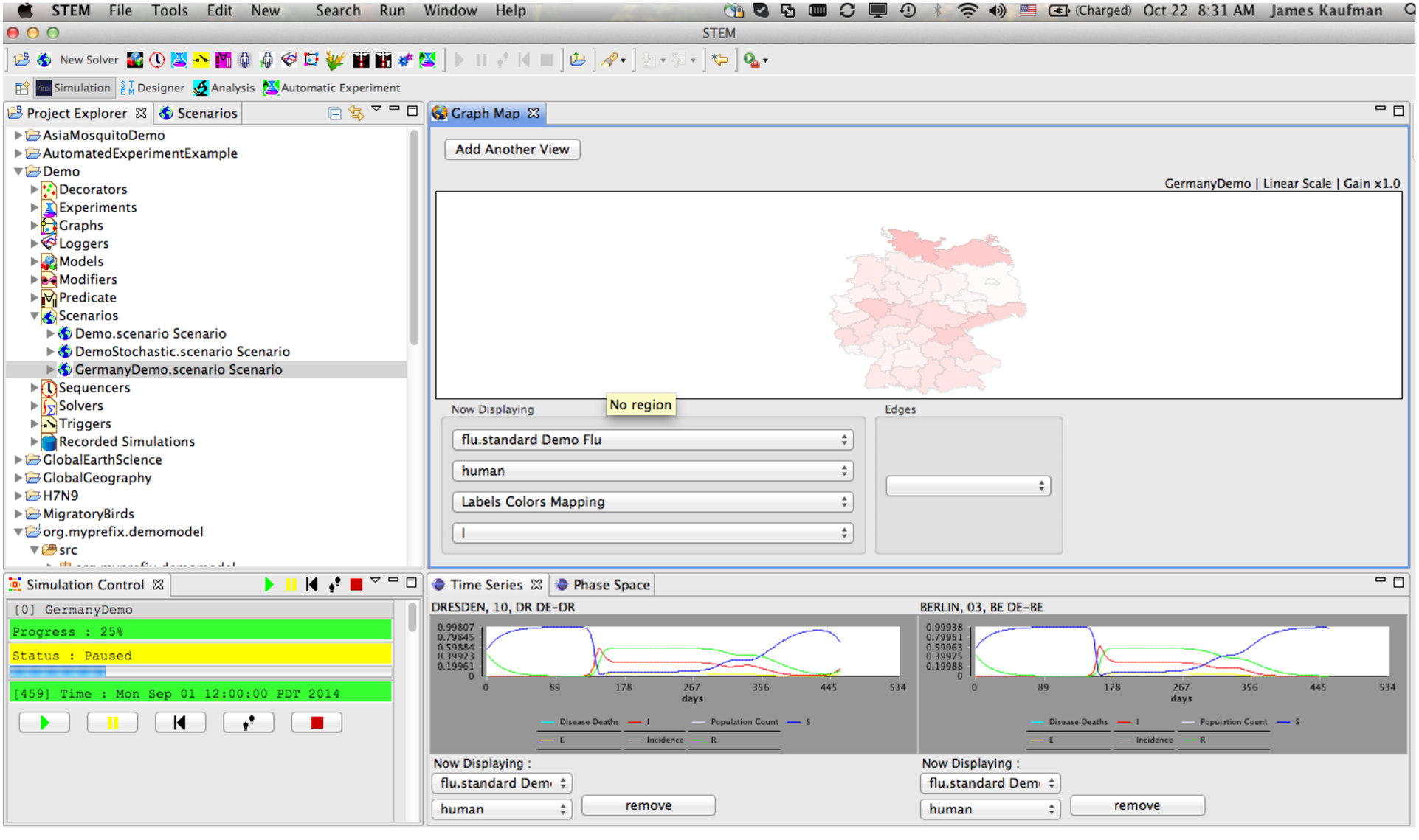



```
/**
 * Computes delta for transition s -> e
 * @generated
 */
protected double s_e (double t, long timeDelta, STEMTime time, DemoFlu model, DemoFluLabel label, DemoFluLabelValue labelValue, Node node
double modulation=(1.0)
/(((1.0)
+(Math.exp(
        (0.2)
        *(((CTDLFunctions.temperature(
                node
                        ,
                time
                        ,
                timeDelta
                        ,
                t
                ))
        -(10.0)
        ))
        ))
))
;
return (model.getTransmissionRate())
*(labelValue.getS())
*(org.eclipse.stem.diseasemodels.functions.CTDLFunctions.computeEffective(
        (org.eclipse.stem.diseasemodels.standard.StandardPackage.eINSTANCE.getSILabelValue_I())
                ,
        model
                ,
        node
                ,
        label
        ))
*(modulation)
;
}
/**
 * Computes delta for transition e -> i
 * @generated
```

# Results


- Reduced Lines of Code
  - 1000 LOC -> 5 LOC for simple SEIR model
- Improved Performance by generating optimal performance code
  - Temporal Caching
  - Appropriate Data Structures
  - Eliminating primative boxing/unboxing
- Correctness
  - Visual Editor makes compartments, transitions obvious
  - User can define meaning of parameters, … right at the beginning

# Generated Plug-in is hot injected and available at runtime



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# Thank you for your attention


Matthias Filter and the
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