

# *Chemical Supply Chain and Resilience Project*

## *FY 2010 Workshop*

### **The N-ABLE™ Simulation Environment**

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U.S. Department of Homeland Security  
Science and Technology Directorate



## Flexible, High-Performance, Repeatable Simulation Platform

**Computer Scientists work side-by-side with Domain Experts**

**Methodological Best Practices**



# Simulation Software Contributors



**Brian Jones**



**Eric Eidson**



**Greg Mackey**



**John Masciantoni**



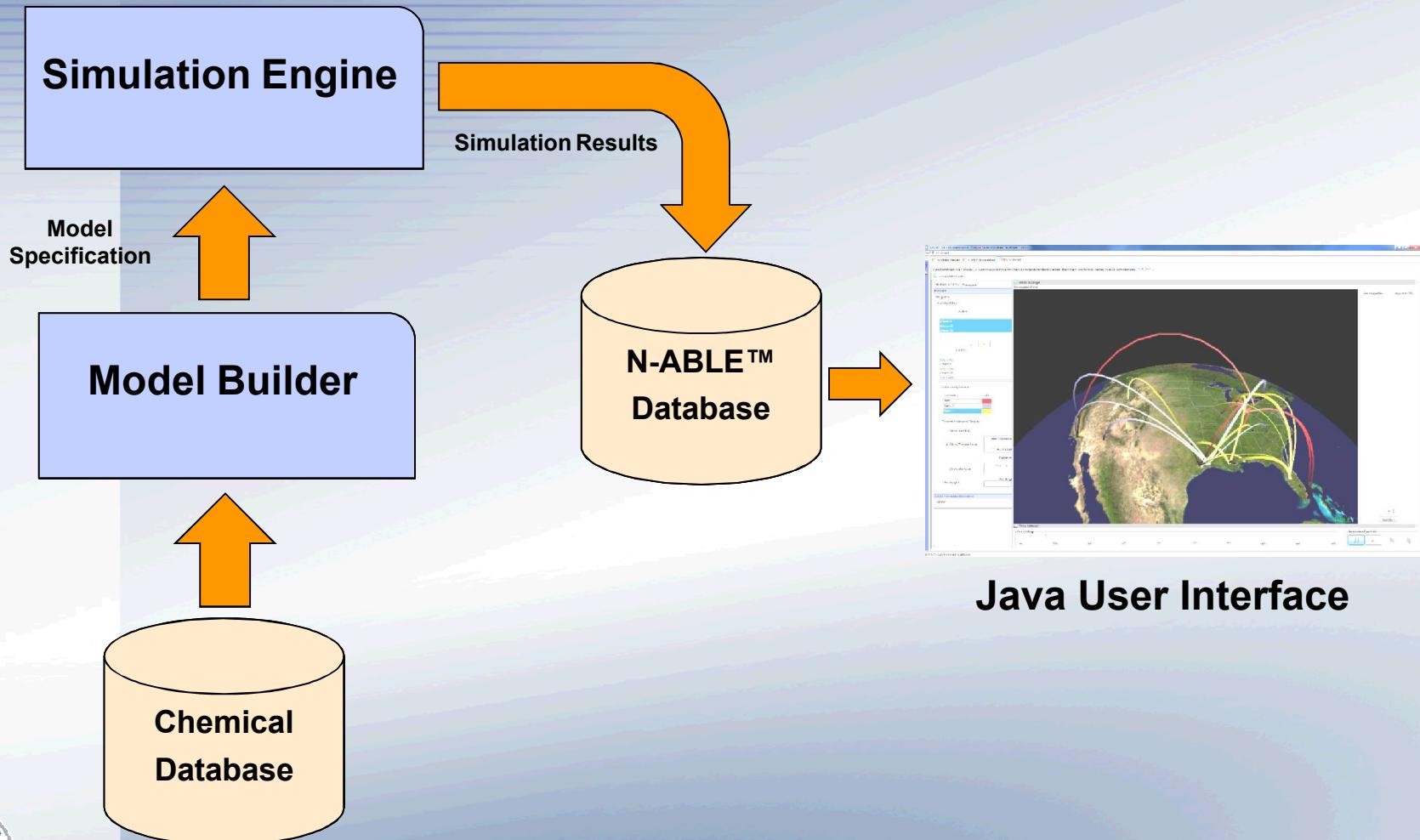
**Roger Mitchell**



**Mark Ehlen**

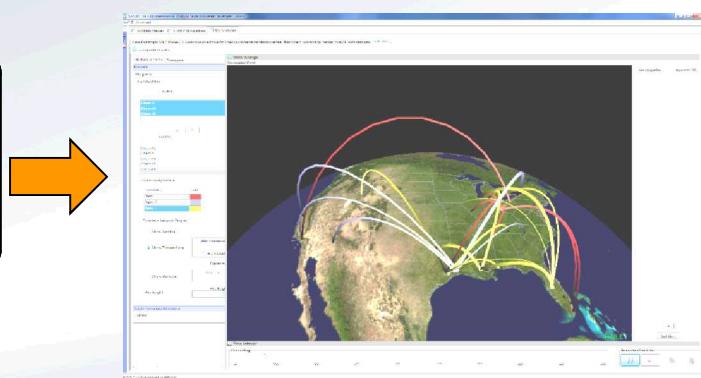
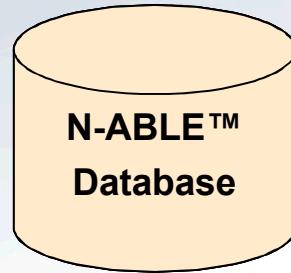
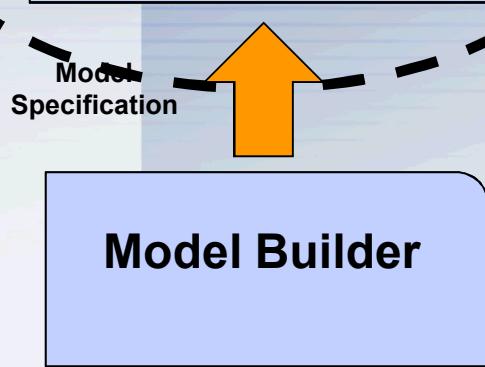
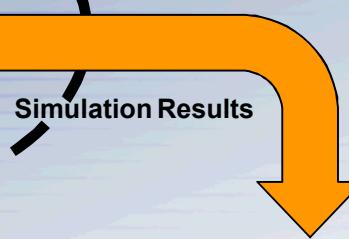
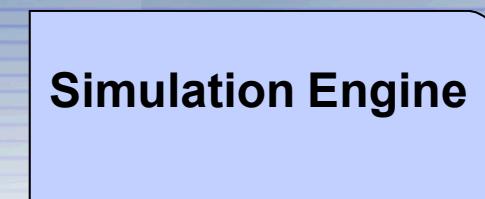


# Architecture

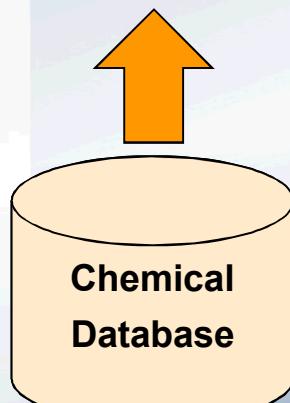


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# Section: Simulation Engine



**Java User Interface**



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# Simulation Engine

## ■ Object-Oriented Discrete Event Engine

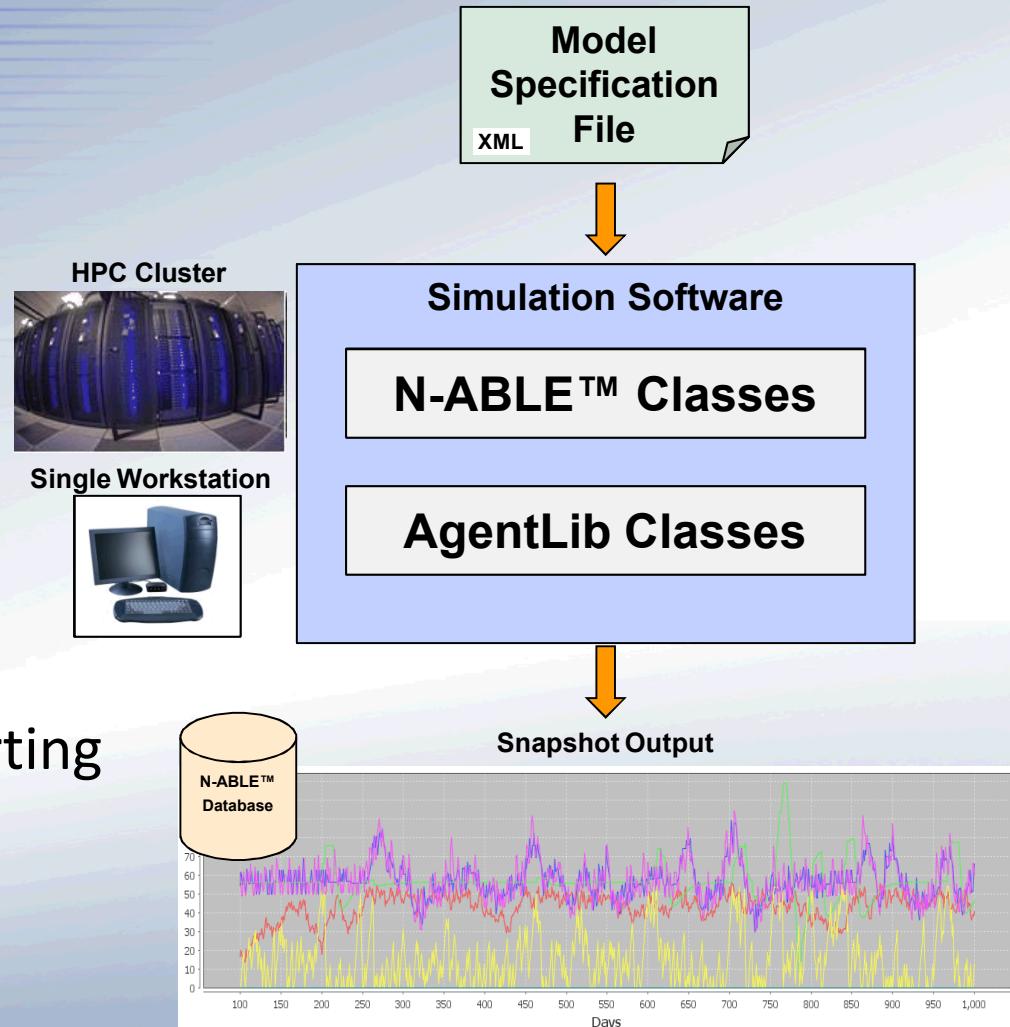
## ■ High Performance

- MPI Parallelism
- Multi-core / HPC

## ■ Repeatable

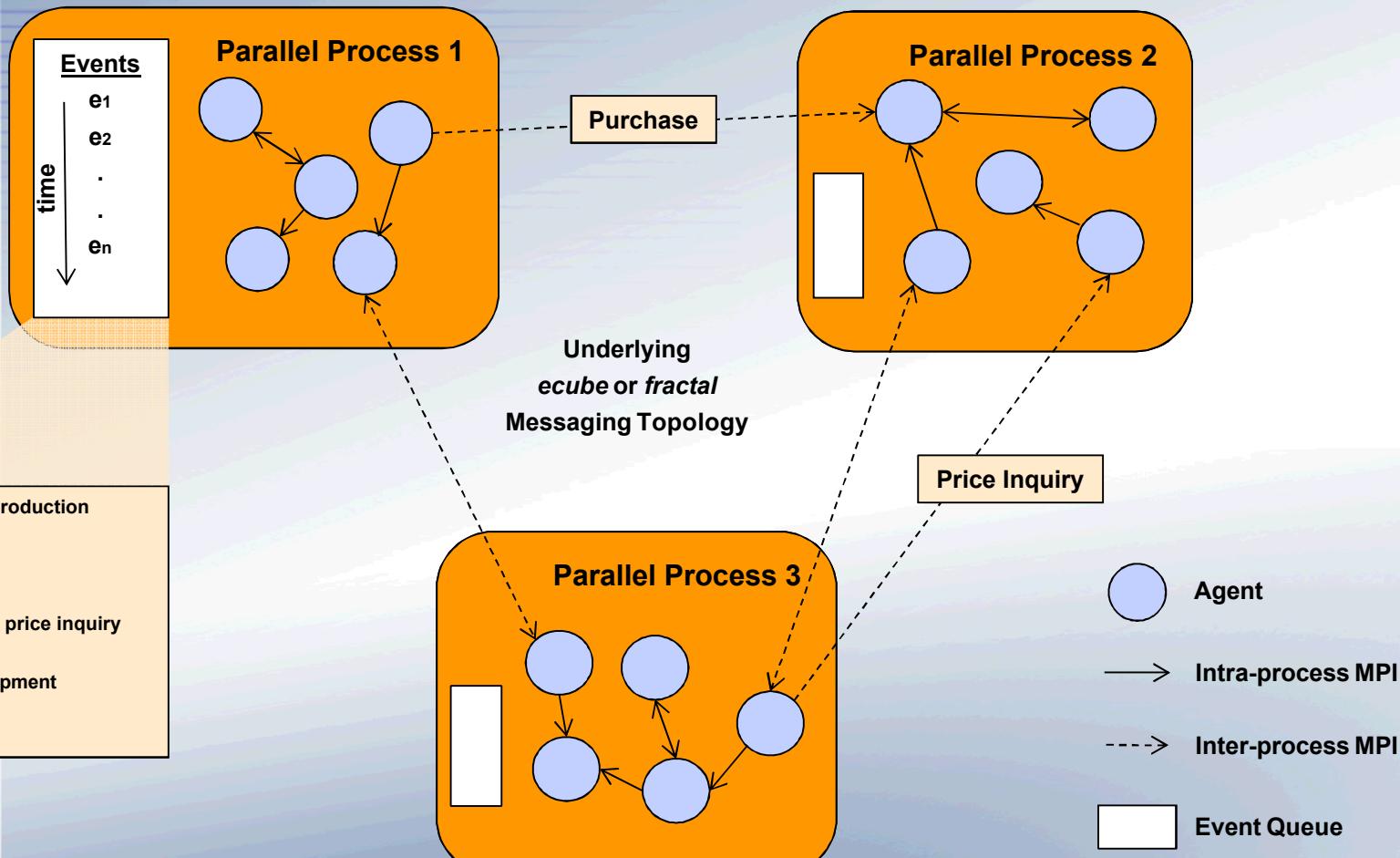
- Stochastic aspects but reproducible given same starting seed

## ■ Portable



# Parallelism

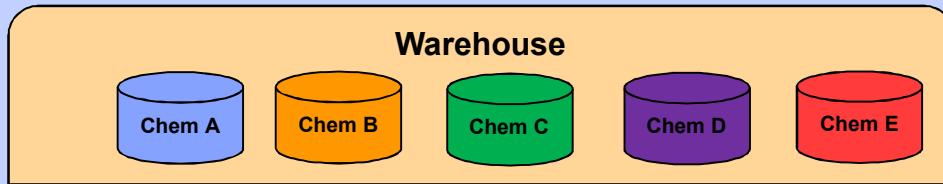
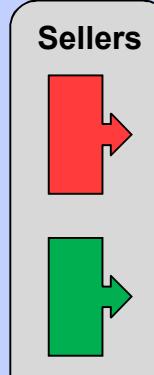
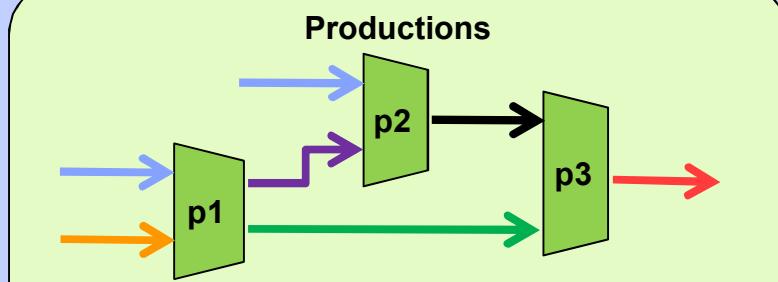
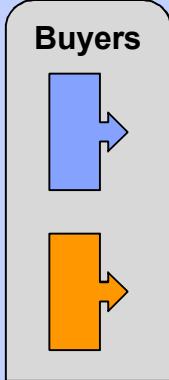
Parallel Processing allows N-ABLE™ to scale to meet problem needs



# Object Structure / Define File

- Object structure mirrors the Model
- Modular design allows pluggable strategies

## Chemical Plant Economic Agent

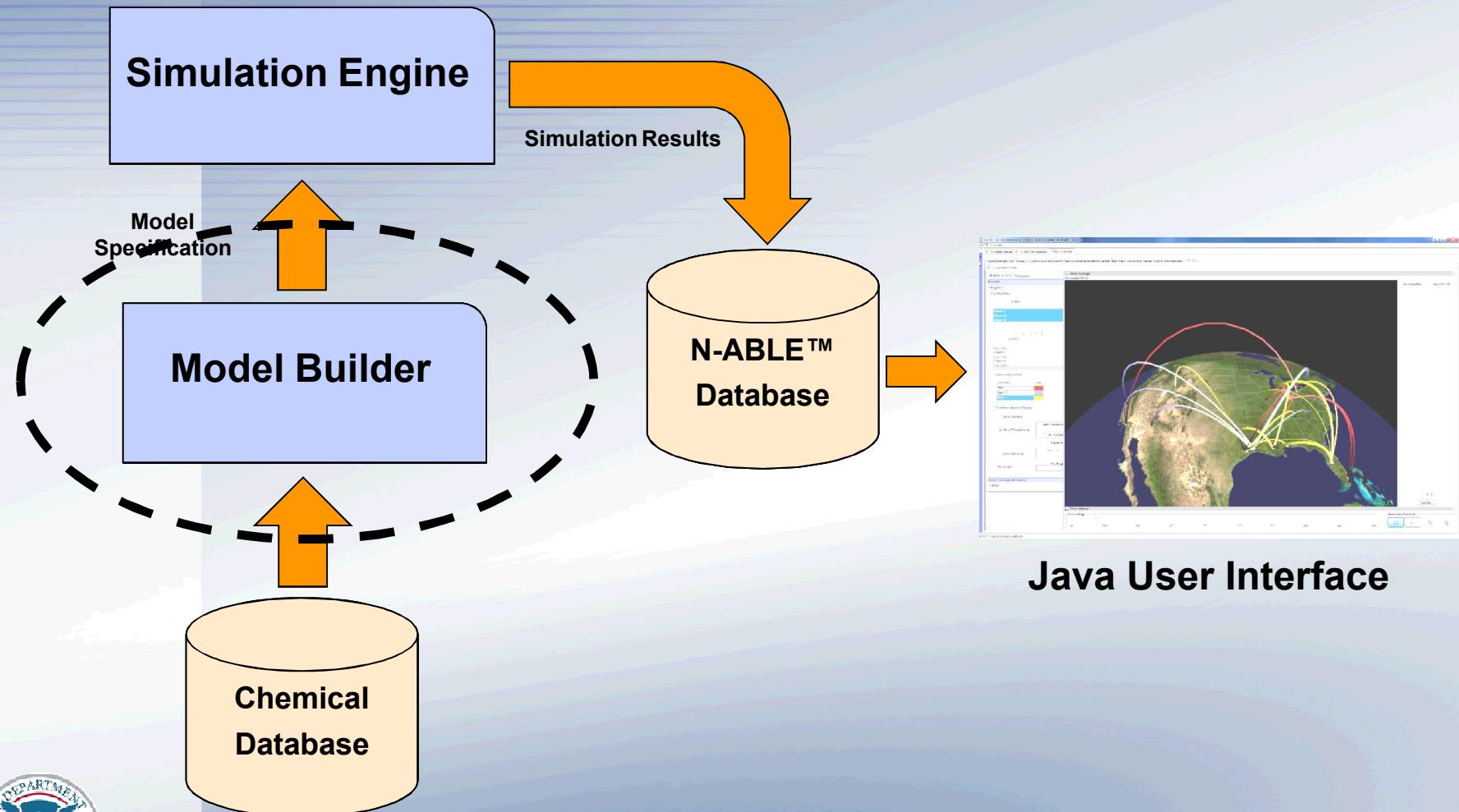


## XML Model Specification, Simplified Snippet

```
<EconomicAgent name="ChemPlant_1">
  <ProductionSleepPeriods/>
  <Location longitude="-95" latitude="30" />
  <InvBasedProdManager>
    <Buyers>
      <FirmBuyer commodity="Chem A"/>
      <FirmBuyer commodity="Chem B"/>
    </Buyers>
    <Sellers>
      <FirmSeller commodity="Chem C"/>
      <FirmSeller commodity="Chem E"/>
    </Sellers>
    <Productions>
      <Producer maxDailyBatches="30" label="p1">
        <ProductionRecipe>
          <Inputs>
            <Input commodity="Chem A" amount="0.7"/>
            <Input commodity="Chem B" amount="2"/>
          </Inputs>
          <Outputs>
            <Output commodity="Chem C" amount="1.5"/>
            <Output commodity="Chem D" amount="1.2"/>
          </Outputs>
        </ProductionRecipe>
      </Producer>
      ...
    </Productions>
    <ProductionChain>
      <Links>
        <Link to="p2" from="p1" commodity="Chem D"/>
        <Link to="p3" from="p1" commodity="Chem C"/>
      </Links>
    </ProductionChain>
  </InvBasedProdManager>
  <InitialStock>
    <Stock minAcceptable="100" maxCapacity="3000" commodity="Chem A" amount="500"/>
    <Stock minAcceptable="300" maxCapacity="5000" commodity="Chem B" amount="1000"/>
  </InitialStock>
</EconomicAgent>
```



# Section: Model Builder



# Model Builder

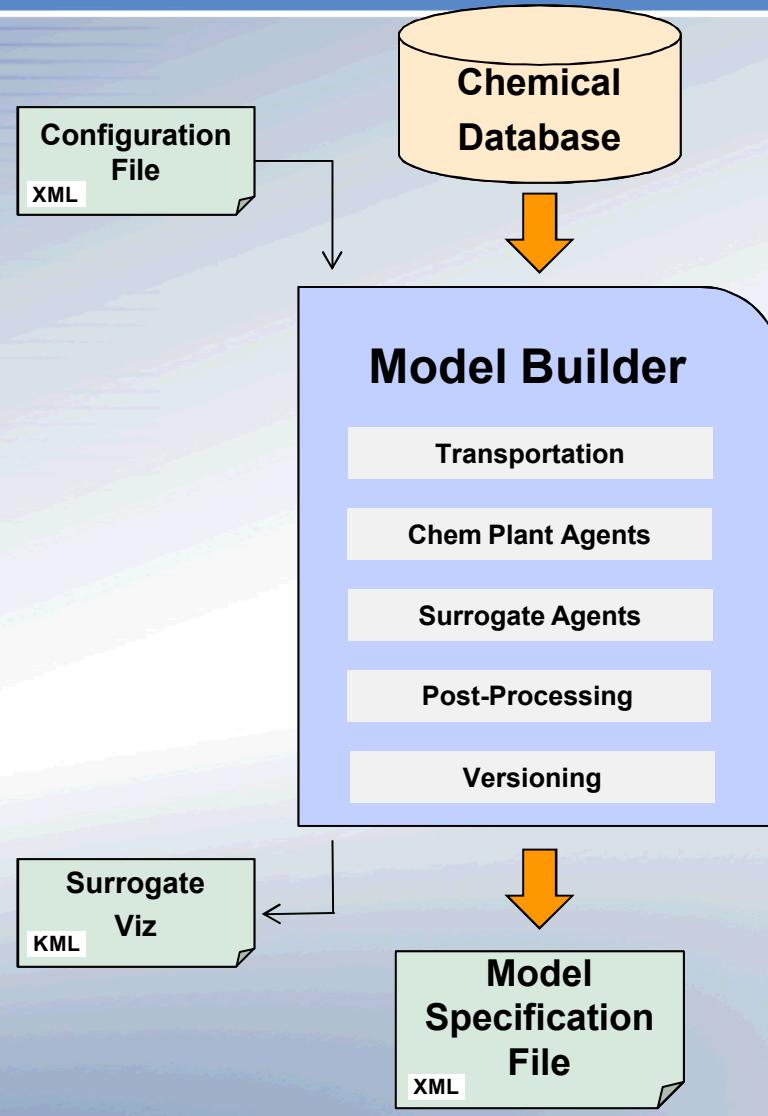
- Turns CDM data into N-ABLE™ model specification

- Modular Processing Pipeline

- File-based Configuration

- Captures Version Info

- Software versions
- Data versions



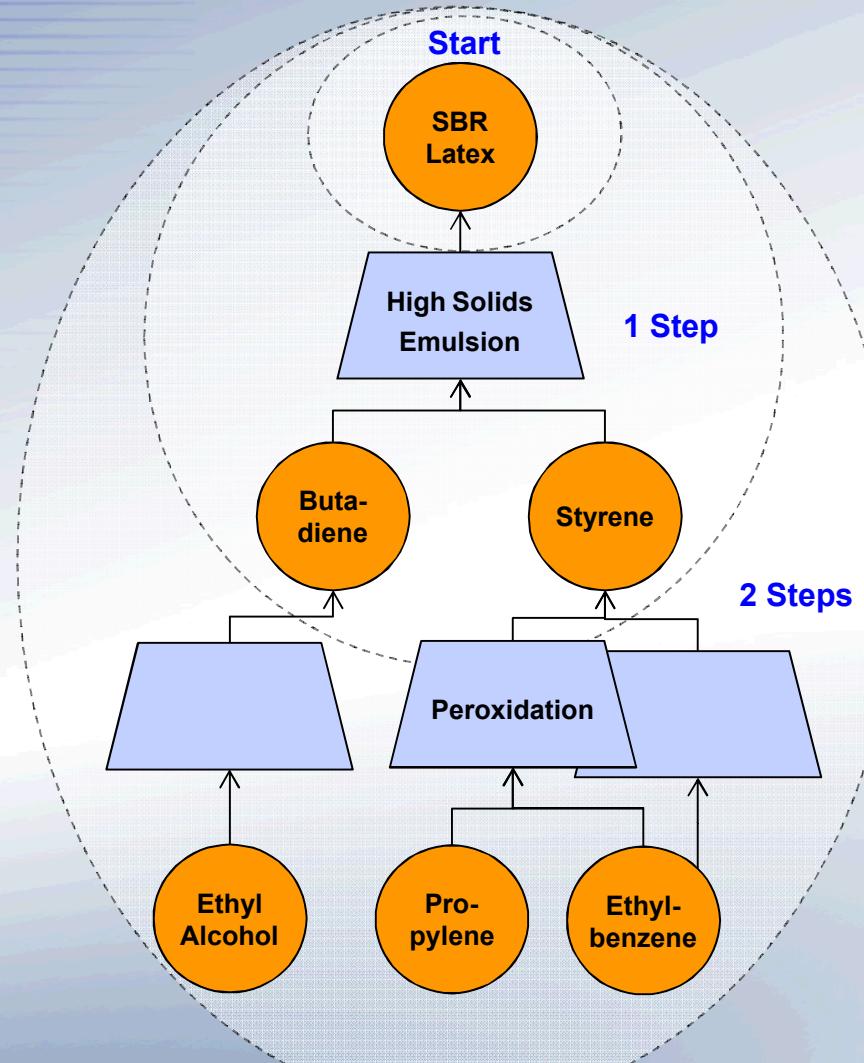
## Process Graph Traversal

### ■ Input:

- Starting chemicals
- # of Steps

### ■ Output:

- Chemicals and Processes connected to starting set
- List of plants that utilize the processes



\* Graph simplified for clarity

# Model Builder

## Builder Configuration File

```
<?xml version="1.0" encoding="UTF-8"?>
```

```
<modelbuilder-config>
```

```
<!-- =====  
 DATA AND SIM SETTINGS  
 ===== -->
```

**Database settings**

**Chemical graph traversal settings**

**Simulation duration, snapshot settings, etc.**

```
<!-- =====  
 AGENT CONFIG  
 ===== -->
```

**Buyer/Seller exceptions**

**Plant Agent behavioral settings**

```
<!-- =====  
 SURROGATE CONFIG  
 ===== -->
```

**Supply/ Demand augmentation**

**Surrogate Agent behavioral settings**

```
<!-- =====  
 TRANSPORTATION  
 ===== -->
```

**Network or simpler 'straight line' shipping**

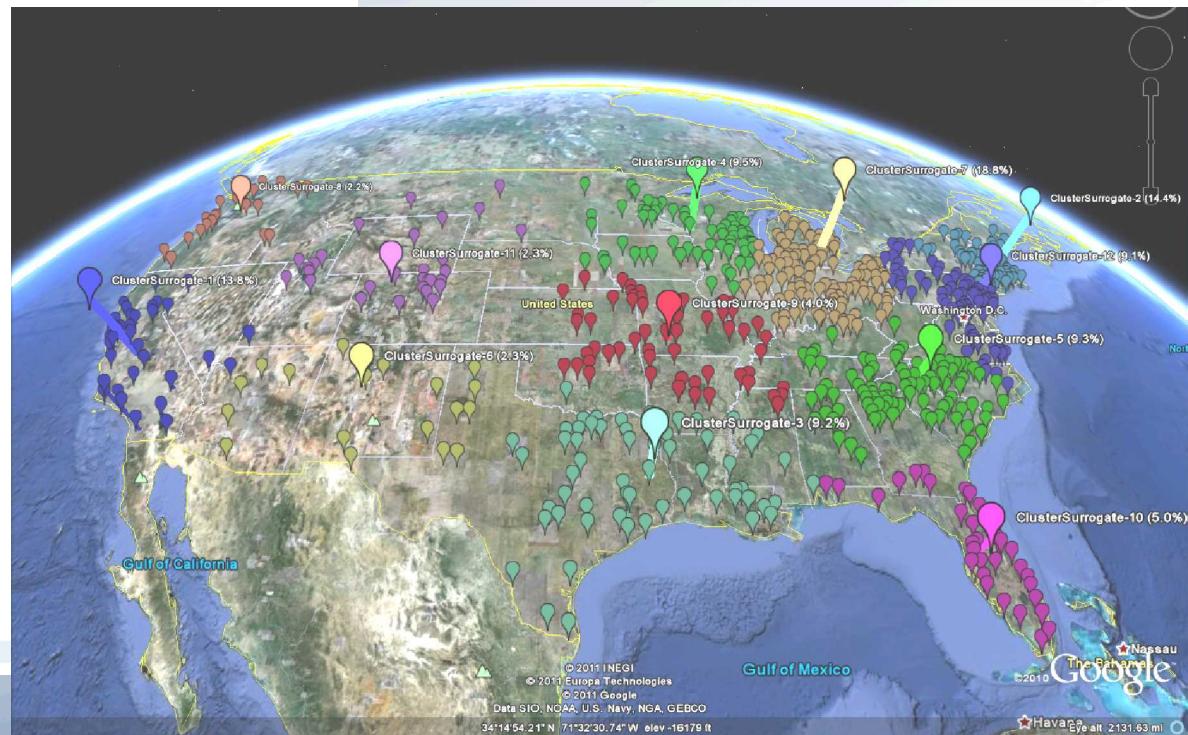
**Network settings (rail, truck, water, etc.)**

```
</modelbuilder-config>
```

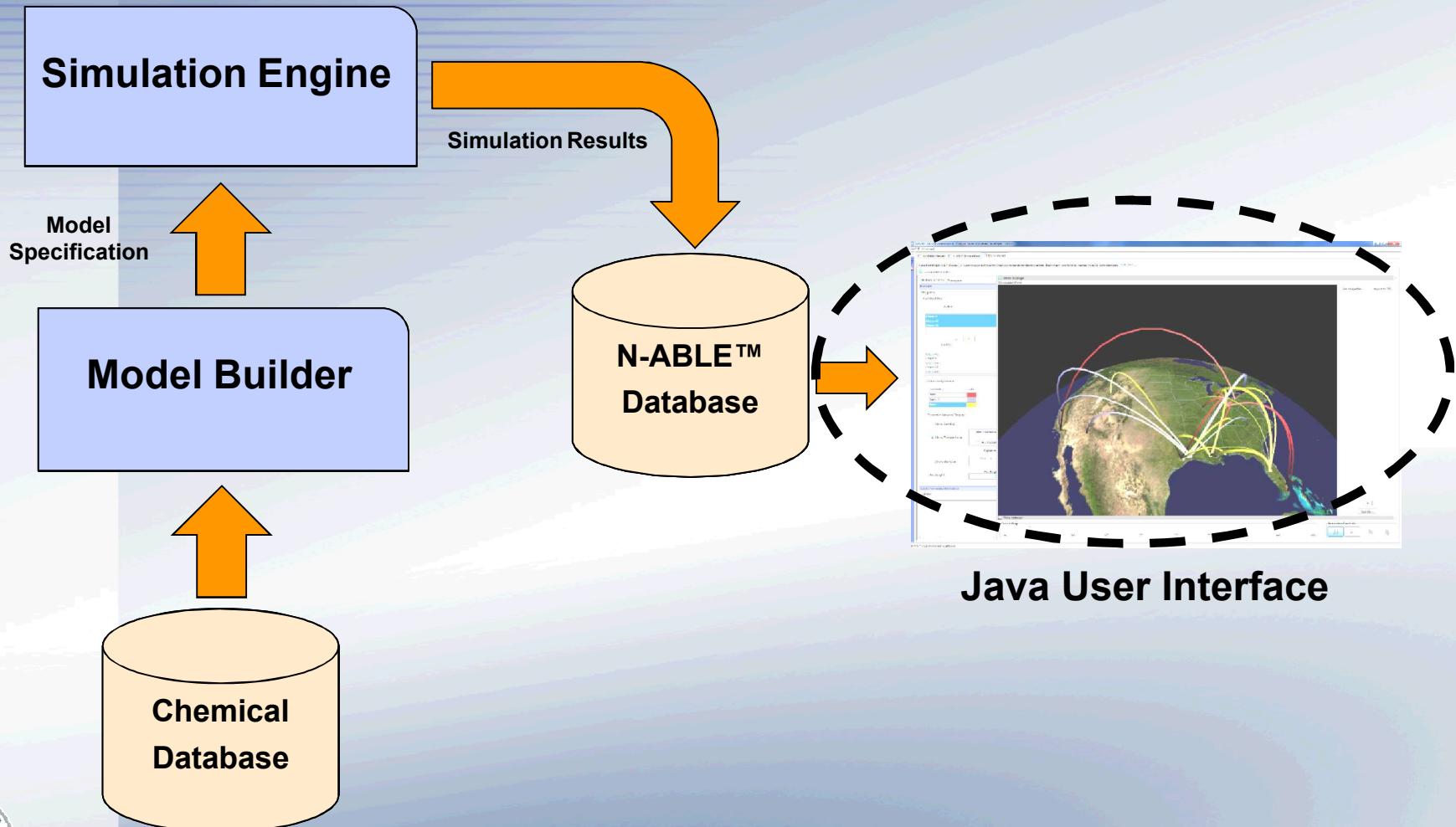


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## Chemical Demand, Spatial Clustering



# Section: User Interface

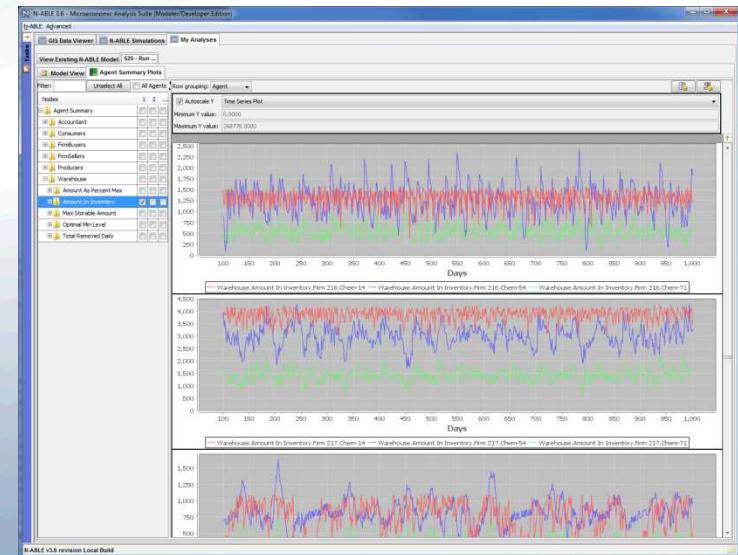
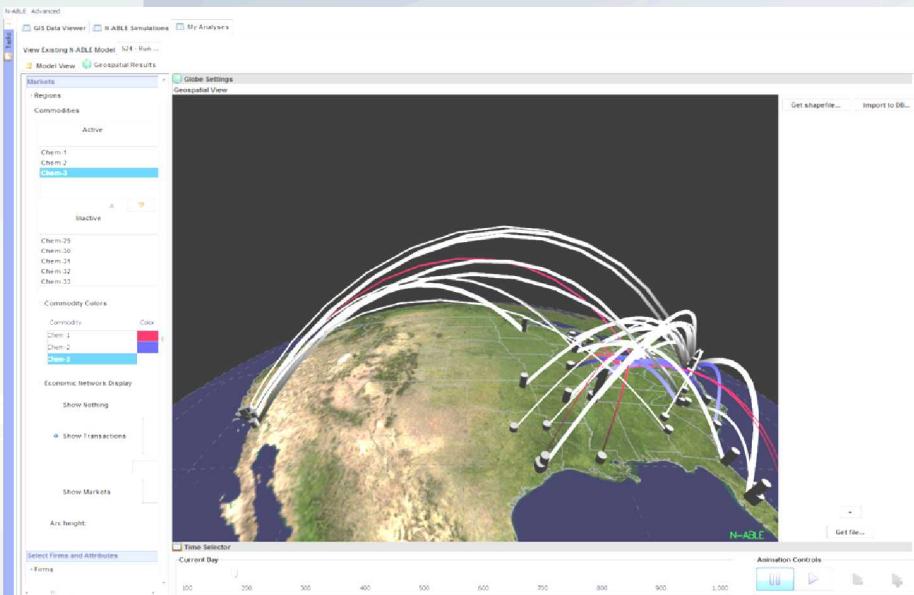


# User Interface

## ■ Supports three main activities:

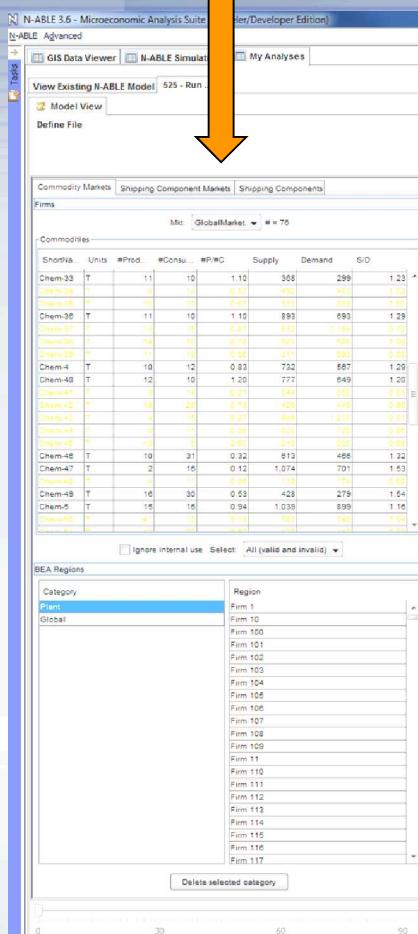
- Pre-sim Model Building and Analysis
- Post-sim Viz and Analysis
- Simulation Archiving, including Baseline/Disruption management

- Portable Java code run via Webstart
- Supports both 2D and 3D visualization via OpenGL

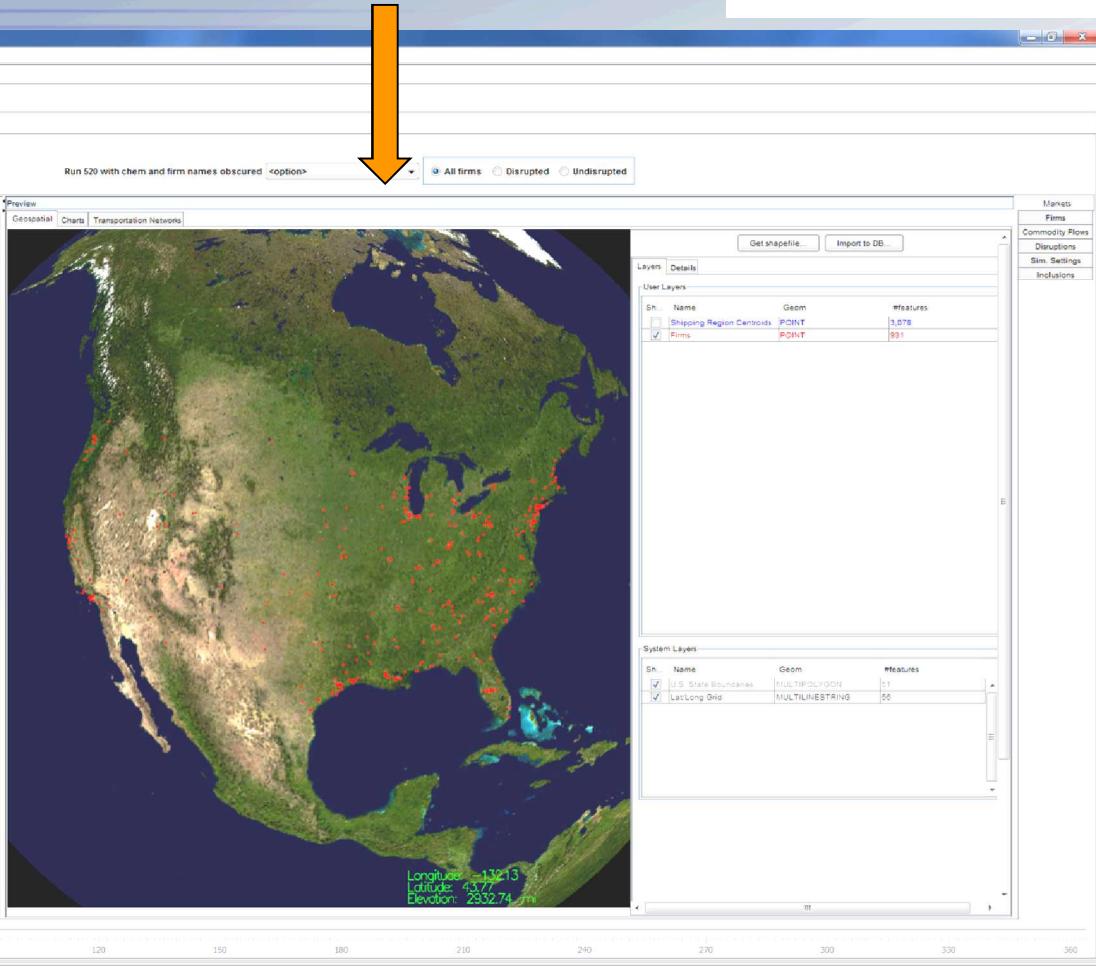


# User Interface: Pre-Simulation

## Overall Market Statistics



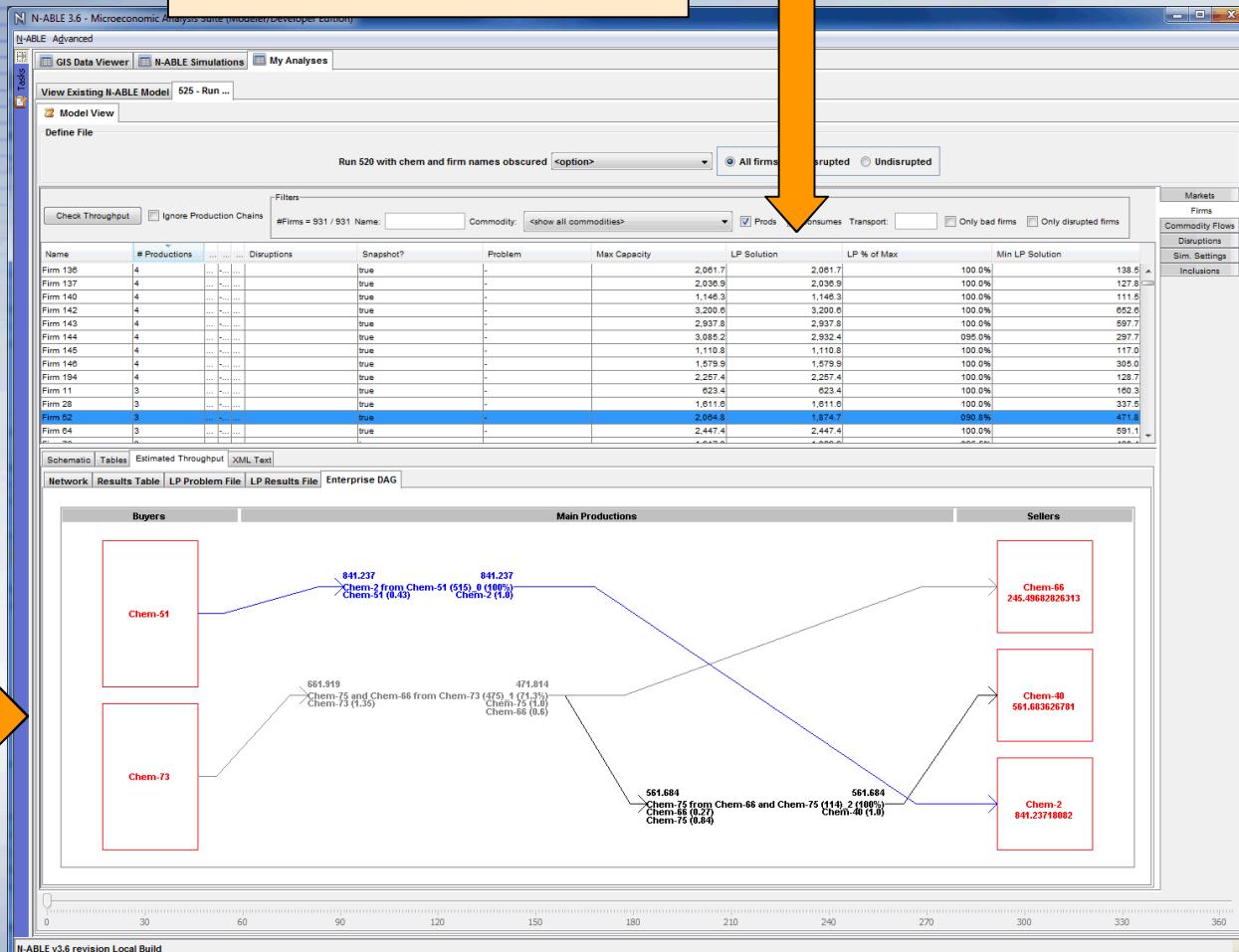
## Geospatial Agent View



# User Interface: Pre-Simulation

## Plant Production Process Checks

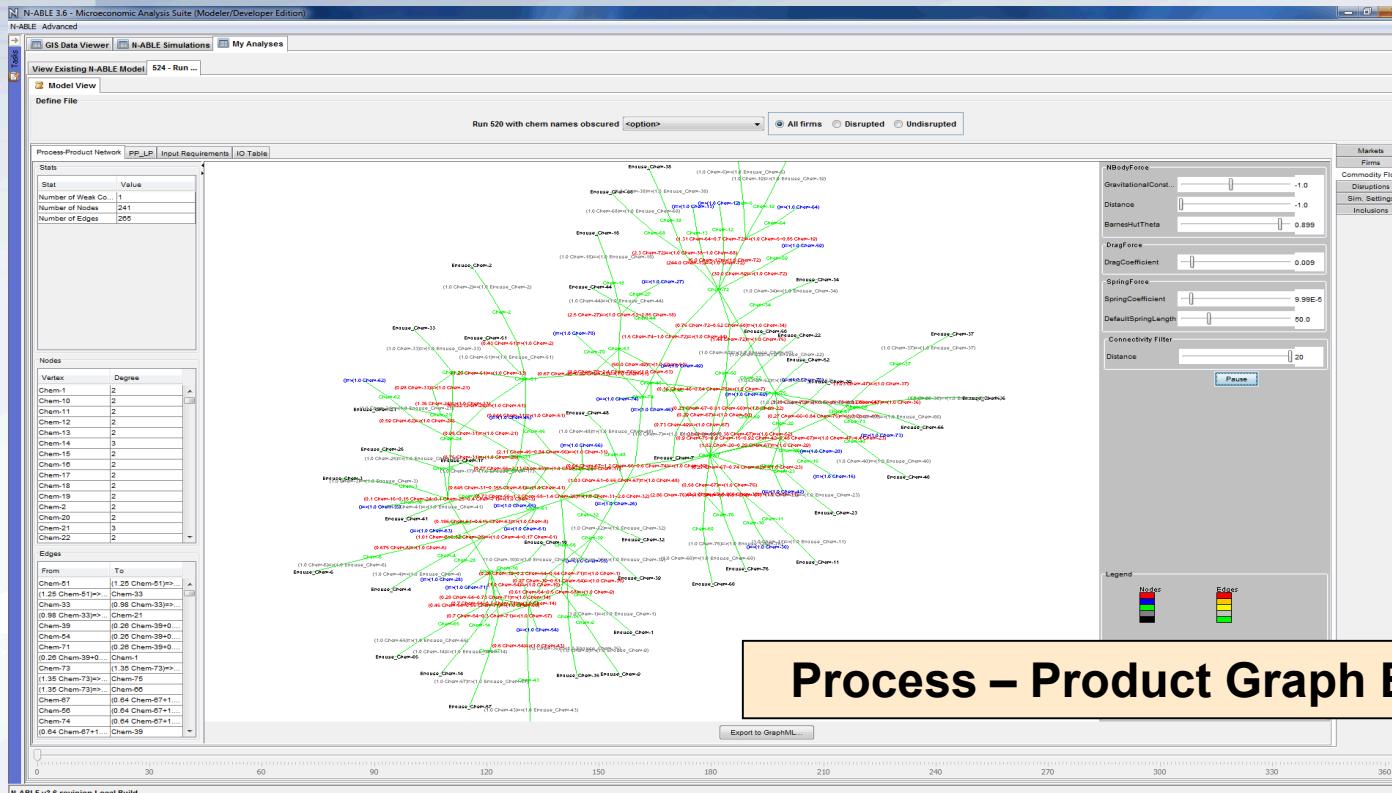
## Firms Tab



# User Interface: Pre-Simulation

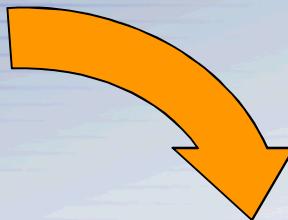
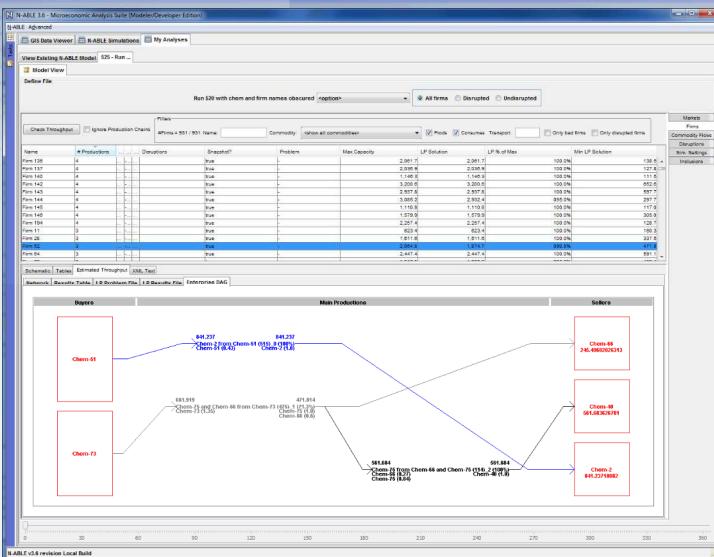
End-to-end throughput checks

Commodity Flows Tab

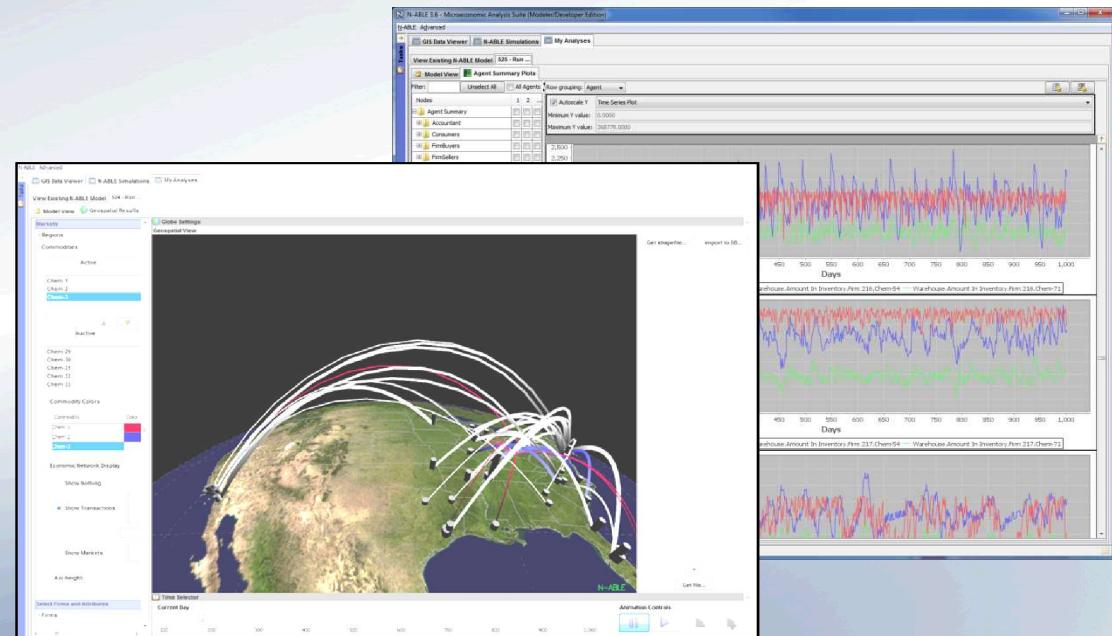


# User Interface

## Pre-Simulation Analysis



## Post-Simulation Analysis



# User Interface: Simulation Archive

Centralized Archive of all Simulations in Database

All inputs are versioned and recorded – traceable and repeatable

GIS Data Viewer   N-ABLE Simulations   My Analyses

Simulations on host: aqua.sandia.gov:9000

Nodes	Node ID	Owner	Description	Submit Time	% Upload	Engine Ver.
gov.sandia.nable.unitTests.Test_Lp1_Producer	284	<testing>	Testing only -single producer produces until warehouse...	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Lp2_TwoIndependentConsumer	285	<testing>	Testing only -two consumers in same agent drawing ...	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Lp2_TwoIndependentProducers	286	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Lp3_OneConsumerWithTwoOutputs	287	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Lp3_ProducerOfTwoOutputs	288	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Lp4_ProductionChain21	289	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Lp6_ProductionChain21	290	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Lp7_TwoSerialChainedProductions	291	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Market	292	<testing>	Testing only -single producer, single consumer	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Market_DualProduction_Inputs	293	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Market_DualProduction_ConstrainedInputs	294	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Market_DualProduction_OneNonBuyingConsumer	295	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Market_DualProduction_WithoutInputs	296	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_CapturedProducerConsumerFirm	297	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_ThreeCapturedProductions	298	<testing>	Testing only -	Jun 7, 2011 17...	100.0	1296
gov.sandia.nable.unitTests.Test_Single_Producer_Disruption	299	testing	Testing only -Single Producer with disruption at 10 to ...	Jun 7, 2011 17...	100.0	1296

Notebook: Setup done.

Simulations can be promoted to “Baseline” status

Baseline simulations can have disruptions applied

GIS Data Viewer   N-ABLE Simulations   My Analyses

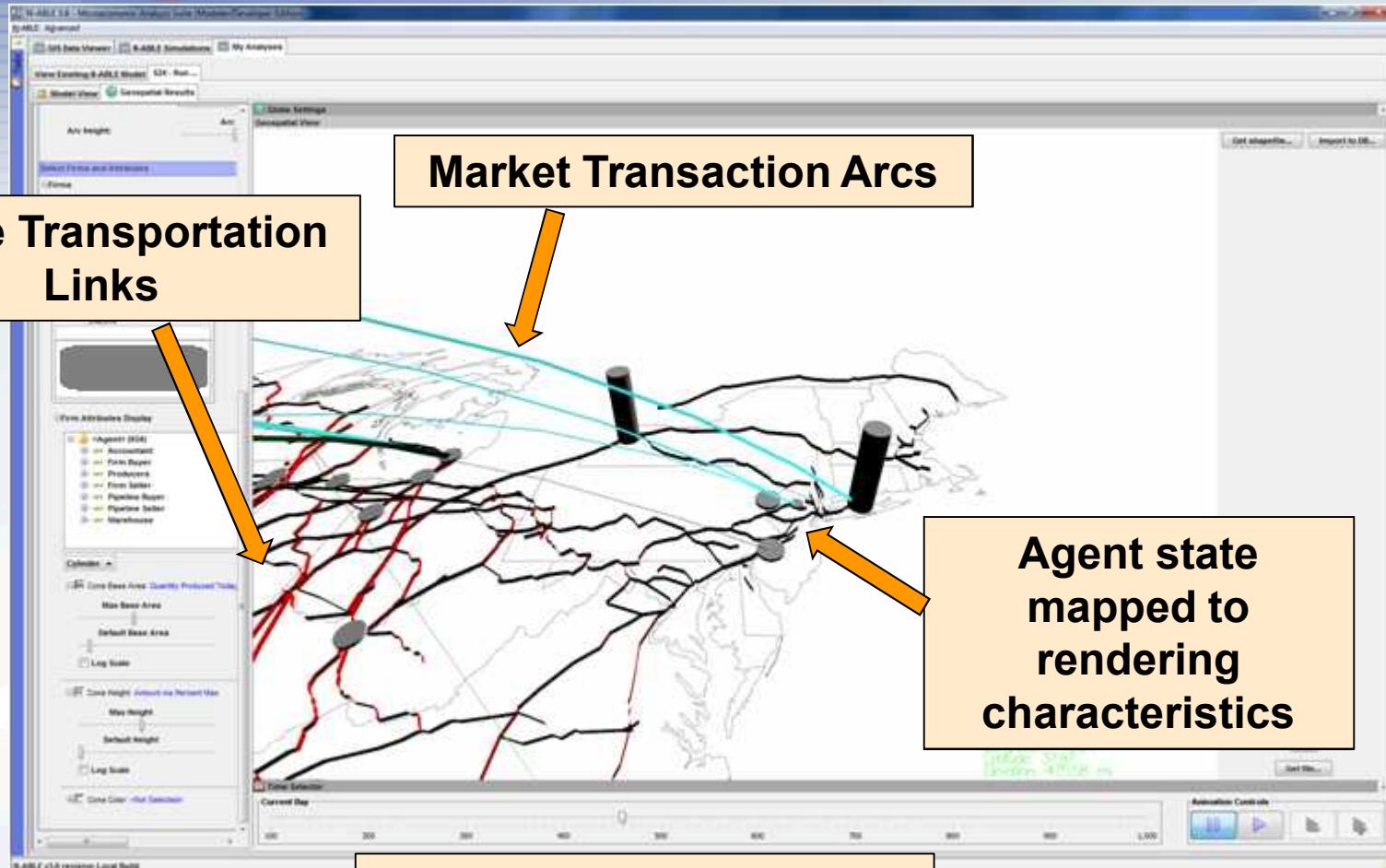
Baselines and Disruptions on host: aqua.sandia.gov:9000

Nodes	N...	Owner	Description	...	...
<b>B</b> Chemical Baseline Model	304	bsjone	Brian's example baseline model for demo purposes	J...	1...
<b>B</b> Petrochemical Model	305	bsjone	U.S. Petrochemical supply chain model	J...	1...
<b>D</b> Petro Katrina Disruption	307	bsjone	Katrina 4 zones, U.S. Petrochemical supply chain model	J...	1...
<b>D</b> Petro New Madrid Disruption	308	bsjone	New Madrid Extensive zone 3 month, U.S. Petrochemical supply chain m...	J...	1...
<b>B</b> Petrochemical / Plastics / Ag Model	306	bsjone	U.S. Petrochemical / Plastics / Agriculture supply chain model	J...	1...
<b>D</b> Petro/Ag New Madrid multi-zone Disruption	309	bsjone	NM Complete Zone, NM Ext Zone, U.S. Petrochemical / Plastics / Agricultu...	J...	1...



# User Interface: Post-Simulation

## Geospatial Simulation Animation



# User Interface: Post-Simulation

## Time Series Visualization - Aggregates

Data Export

Data Selector

- # of Firms Reporting
- Total Distance
- Total Placed Orders
- Total Revenues
- Total Payments
- Cash Flow Statement
- Inventories
- Inventory Capacities
- Average Distance
- Estimated Distance
- Production Capacities
- Net Demand
- Distances
- Distances
- Consumer Surplus
- Production Sold (#)
- Average Last Price Paid
- Unmet Demand
- Outstanding Orders
- Placed Orders
- Production Sold (\$)
- Productions
- Average Estimated Distance
- Shipments

Row =  
Commodity

N-ABLE v3.6 revision Local Build



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# User Interface: Post-Simulation

# Time Series Visualization – Agent Level



## Row = Agent



# User Interface: Disruption Specification

## Damage Contour Library

Add Disruptions

Available Contours

Name
chemical_plant_damage_ge_moderate_wgs84
chemical_plant_damage_zones
chemical_plant_damage_zones_100
chemical_plant_damage_zones_25
chemical_plant_damage_zones_50
chemical_plant_damage_zones_75
<b>dmg_nmsz_day1_3_ep_outage_100_wgs84</b>
dmg_nmsz_day1_3_ep_outage_25_wgs84
dmg_nmsz_day1_3_ep_outage_50_wgs84
dmg_nmsz_day1_3_ep_outage_75_wgs84
dmg_nmsz_day1_3_ep_outage_wgs84

Add selected countour

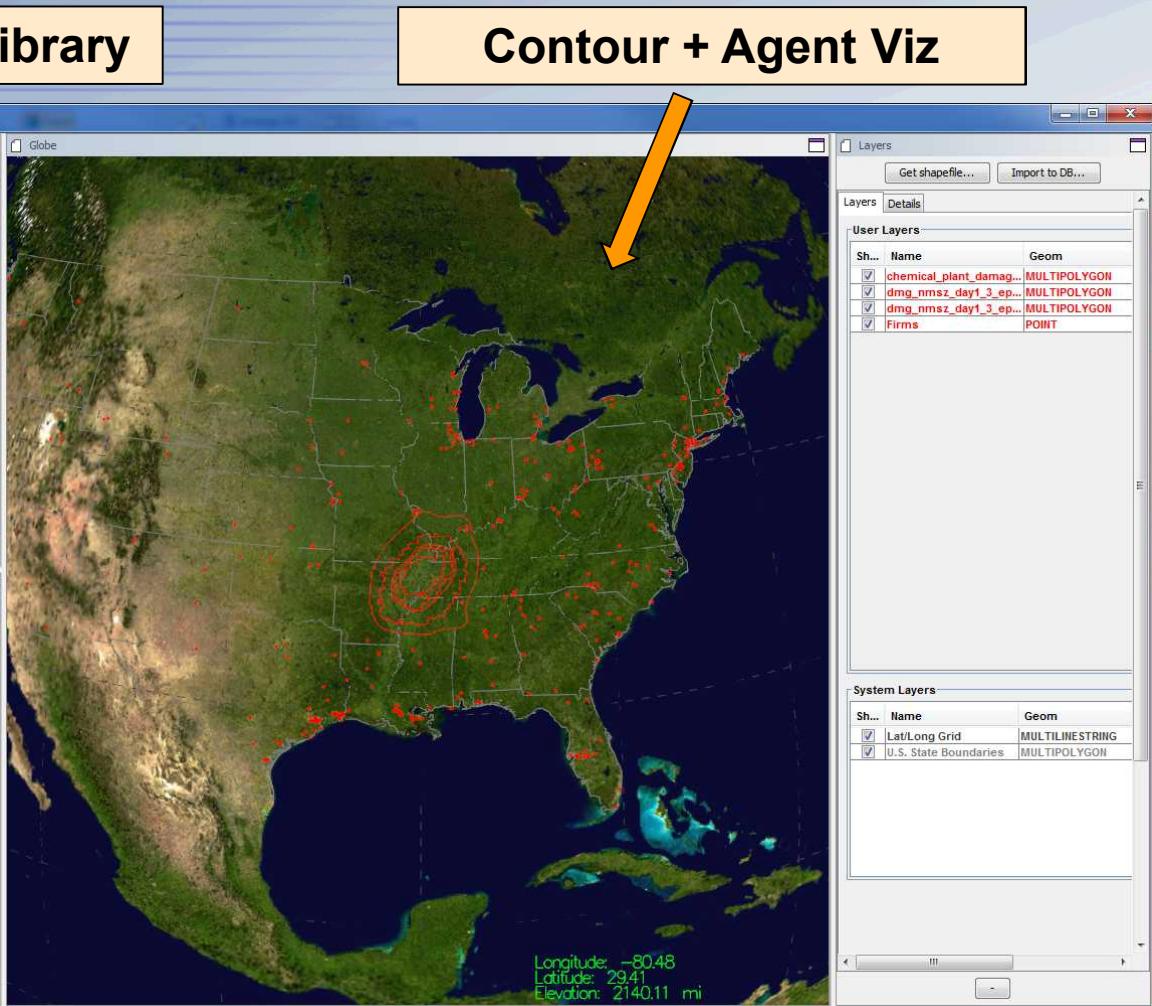
Model Disruptions

Name	Contour	Start Day	Stop Day
NM Seismic zone 1	chemical_plant_damage_zones_25	500	590
EP zone 1	<b>dmg_nmsz_day1_3_ep_outage_50_wgs84</b>	500	530
EP zone 2	dmg_nmsz_day1_3_ep_outage_100_wgs84	500	507

Delete all Run Simulation

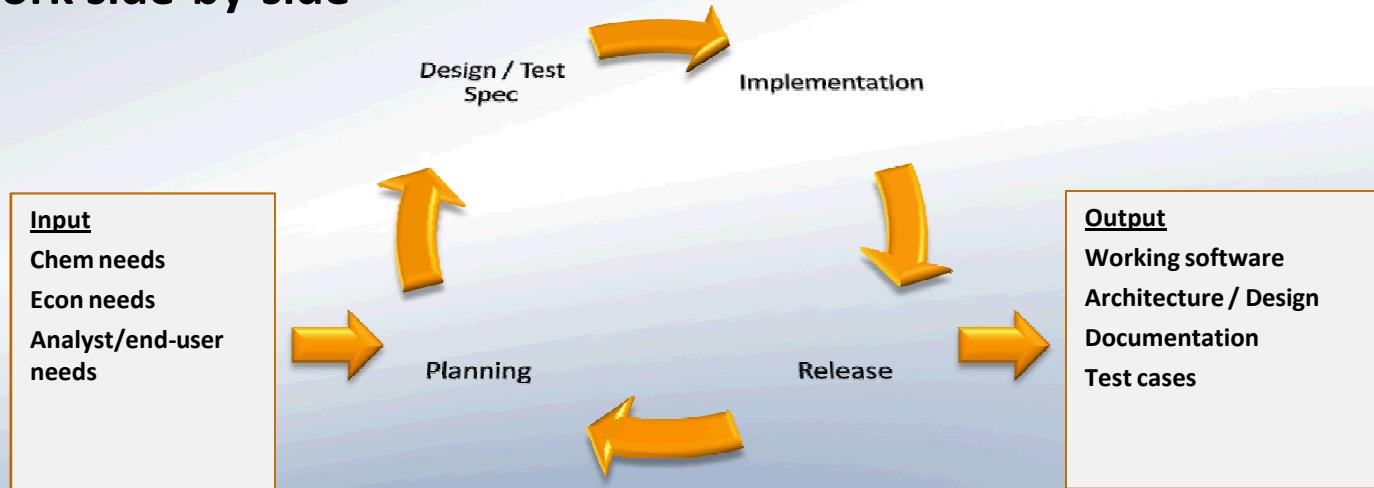
## Scenario Specification

## Contour + Agent Viz



# Software Methodology

- Iterative Development (“Agile”)
- 2-week iterations to adapt as new ideas emerge
- Computer Scientists and Modelers work side-by-side
- Continuous, Automated Build & Test
- Track Defects, Requirements, Task assignments



# Collaboration with TeamForge

- Requirements / Task / Defect Tracking with Prioritization
- Coordination + Traceability
- Documents / Message Board
- Version Control

COLLABNET TeamForge™

Project: N-ABLE

Project Home Tracker Documents Source Code Discussions Reports File Releases Wiki Project Admin

Jump to ID: plan1195 GO

SNL Privacy Notice Support Requests

Logged in as: Brian Jones (bsjone) | LOGOUT | HELP

Artifacts

plan1195 : N-ABLE 3.5 Summary

Name: N-ABLE 3.5  
Description:  
Effort: 0 Est, 0 Rem, 194 Act  
Story Points: 0 Open, 0 Total Status: Closed  
Start Date: 03/09/2011 End Date: 05/18/2011  
File Release: NABLE > N-ABLE 3.5.0

Burndown

Open by priority

Open Vs Closed

Priority: P1: 0, P2: 0, P3: 0, P4: 0, P5: 0, None: 0

Planning Folders Active | All

Root Folder N-ABLE 3.3 N-ABLE 3.4 N-ABLE 3.5

Iteration 1 Iteration 2 Iteration 3

N-ABLE 3.5 All

Priority	Artifact ID	Title	Assigned To	Status	Planned For
1	artf36658	Add ability to augment Buyers and Sellers	Brian Jones	Closed	N-ABLE 3.5 > Iteration 5
2	artf36144	Add Baseline/Disruption view	Roger Mitchell	Closed	N-ABLE 3.5 > Iteration 4
3	artf29264	Add MPI capabilities to Client-Initiated Simulations	John Masciantoni	Closed	N-ABLE 3.5 > Iteration 4



## Flexible, High-Performance, Repeatable Simulation Platform

**Computer Scientists work side-by-side with Domain Experts**

**Methodological Best Practices**



# Backup Slides



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# Simulation Engine

- AgentLib
  - Parallel discrete event simulation engine (PDES)
  - General purpose – can be used for chemical supply chains, social networks, pandemic models, etc.
- N-ABLE™
  - Built on top of AgentLib
  - Special purpose – captures economic concepts and behaviors
- Shared characteristics
  - Portable C++ code
  - Tuned for performance
  - Flexible recording system to capture simulation state at each timestep

