

Chemical Supply Chain and Resilience Project FY 2010 Workshop

The N-ABLE™ Simulation Environment

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July 12, 2011

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Science and Technology Directorate**



Sandia National Laboratories

**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



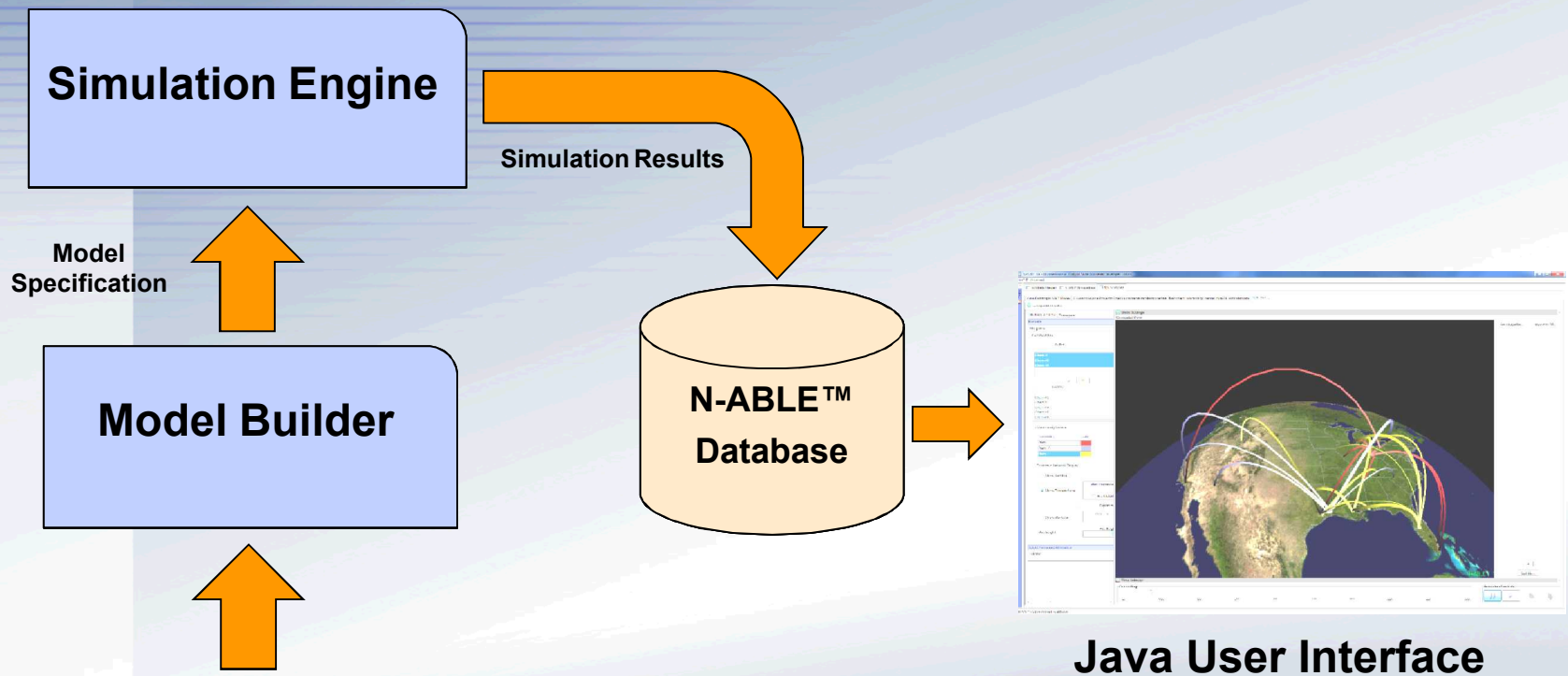
Roger Mitchell



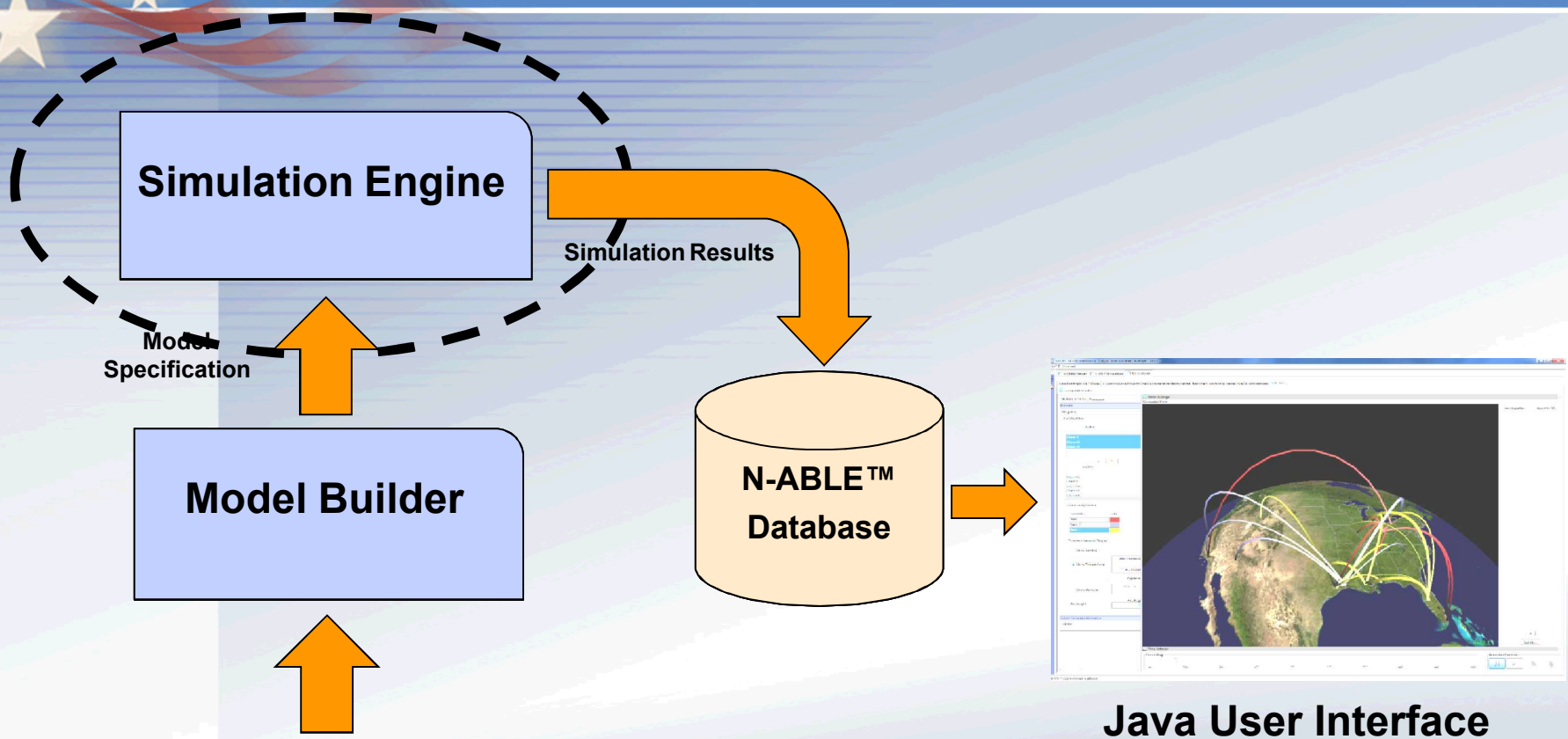
Mark Ehlen



Architecture



Section: Simulation Engine



Simulation Engine

■ Object-Oriented Discrete Event Engine

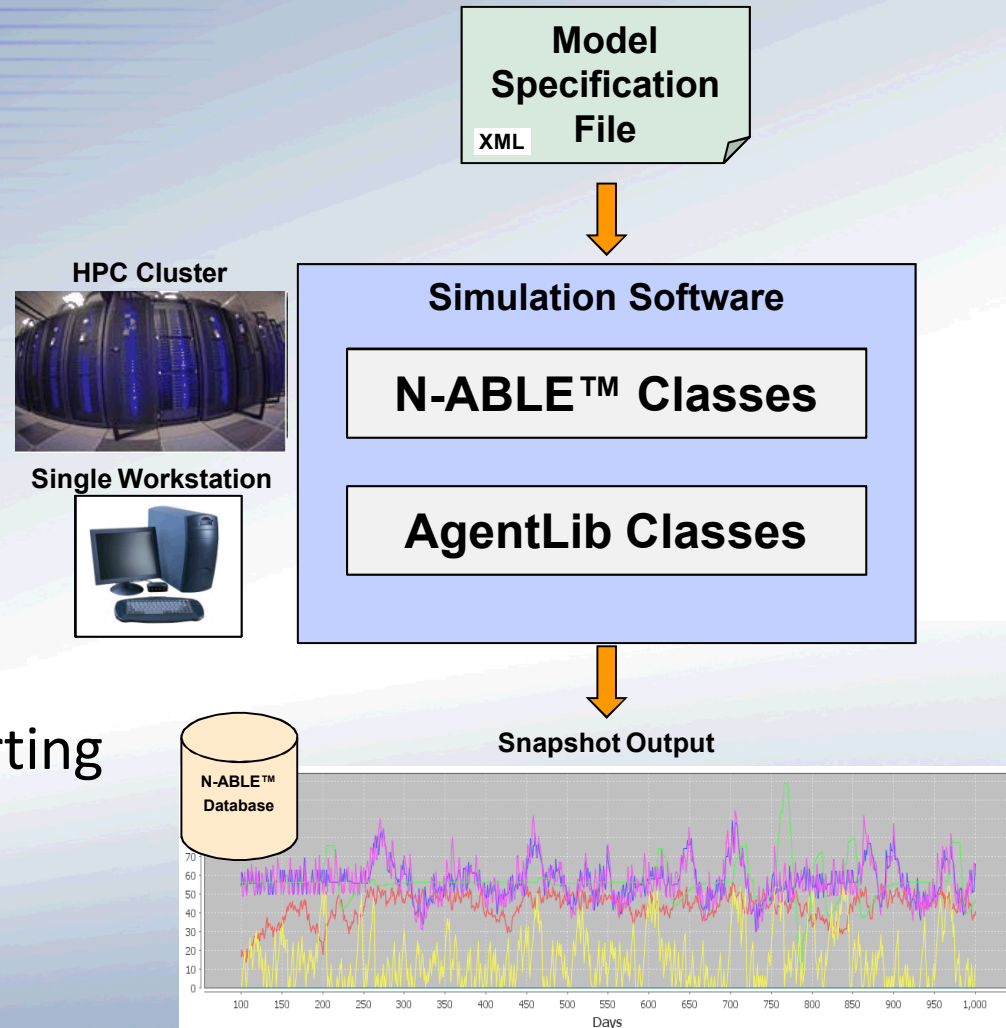
■ High Performance

- MPI Parallelism
- Multi-core / HPC

■ Repeatable

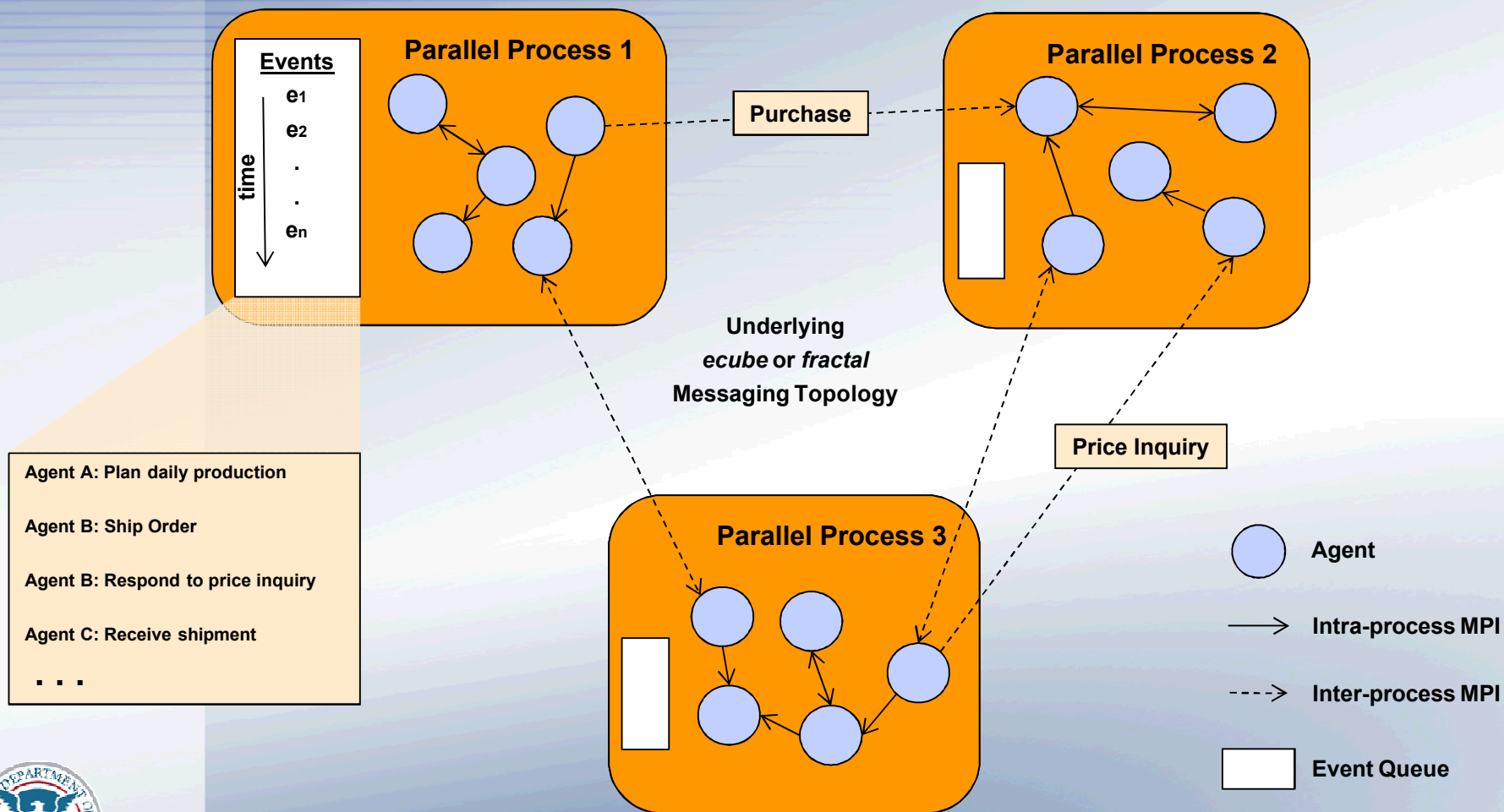
- Stochastic aspects but reproducible given same starting seed

■ Portable



Parallelism

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



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Object Structure / Define File

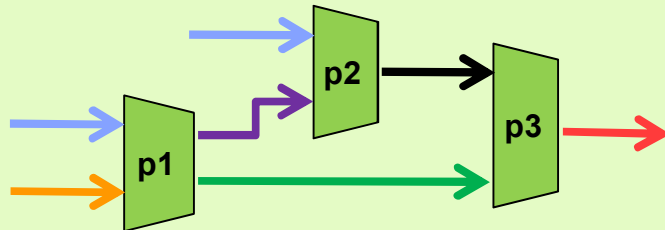
- Object structure mirrors the Model
- Modular design allows pluggable strategies

Chemical Plant Economic Agent

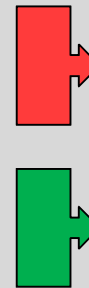
Buyers



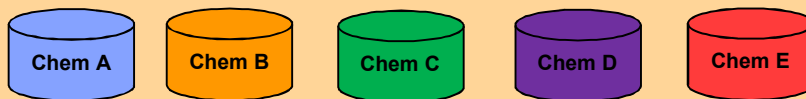
Productions



Sellers



Warehouse

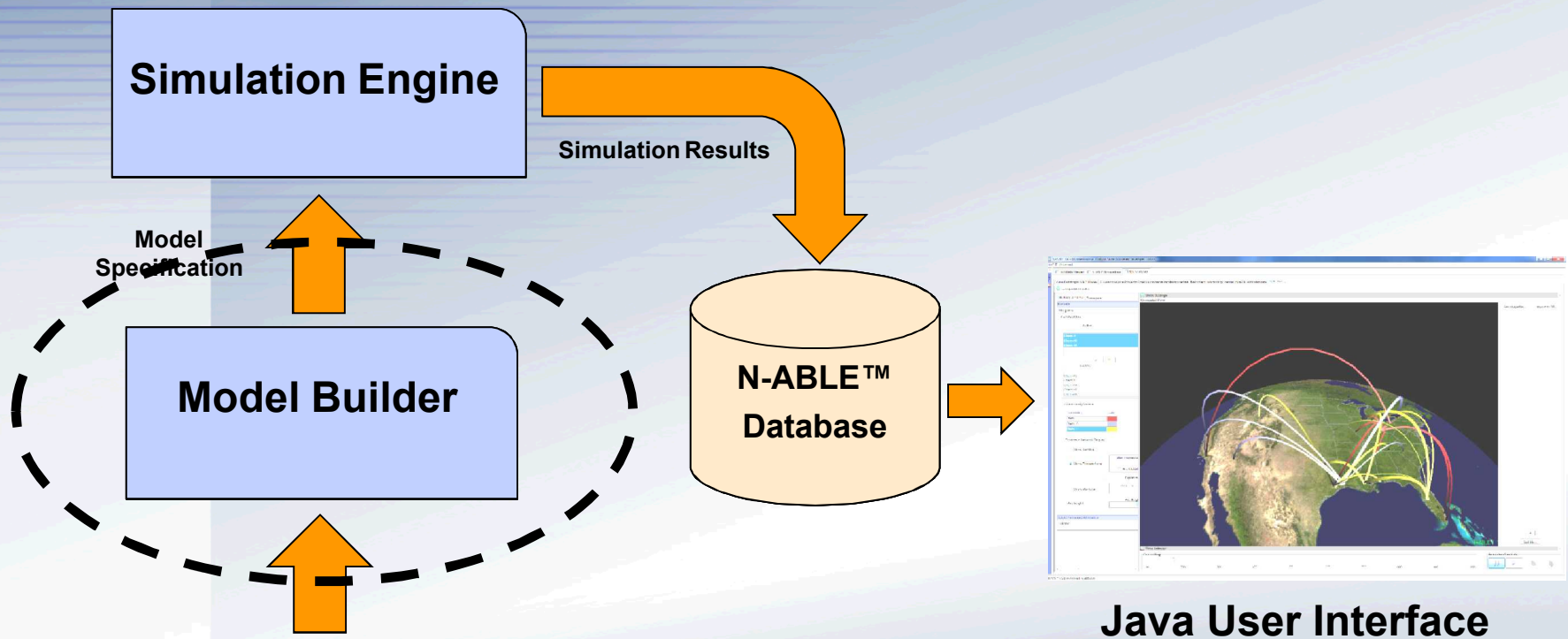


XML Model Specification, Simplified Snippet

```
<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>
```

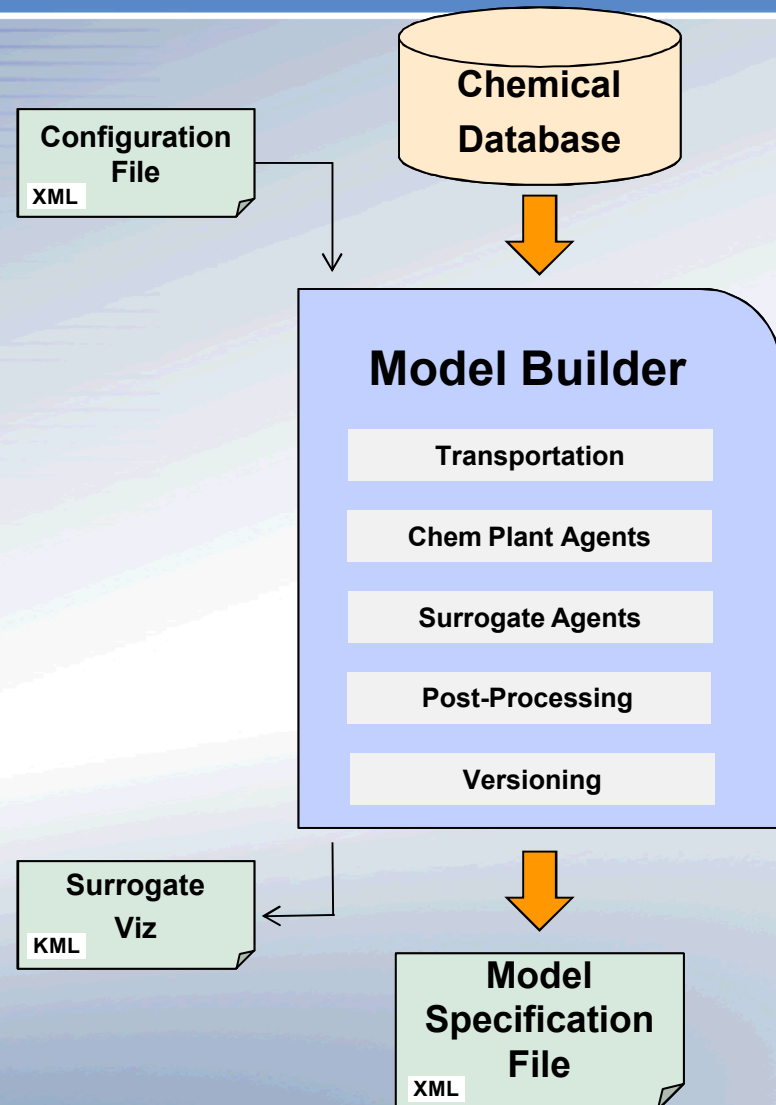


Section: Model Builder



Model Builder

- Turns CDM data into N-ABLE™ model specification
- Modular Processing Pipeline
- File-based Configuration
- Captures Version Info
 - Software versions
 - Data versions



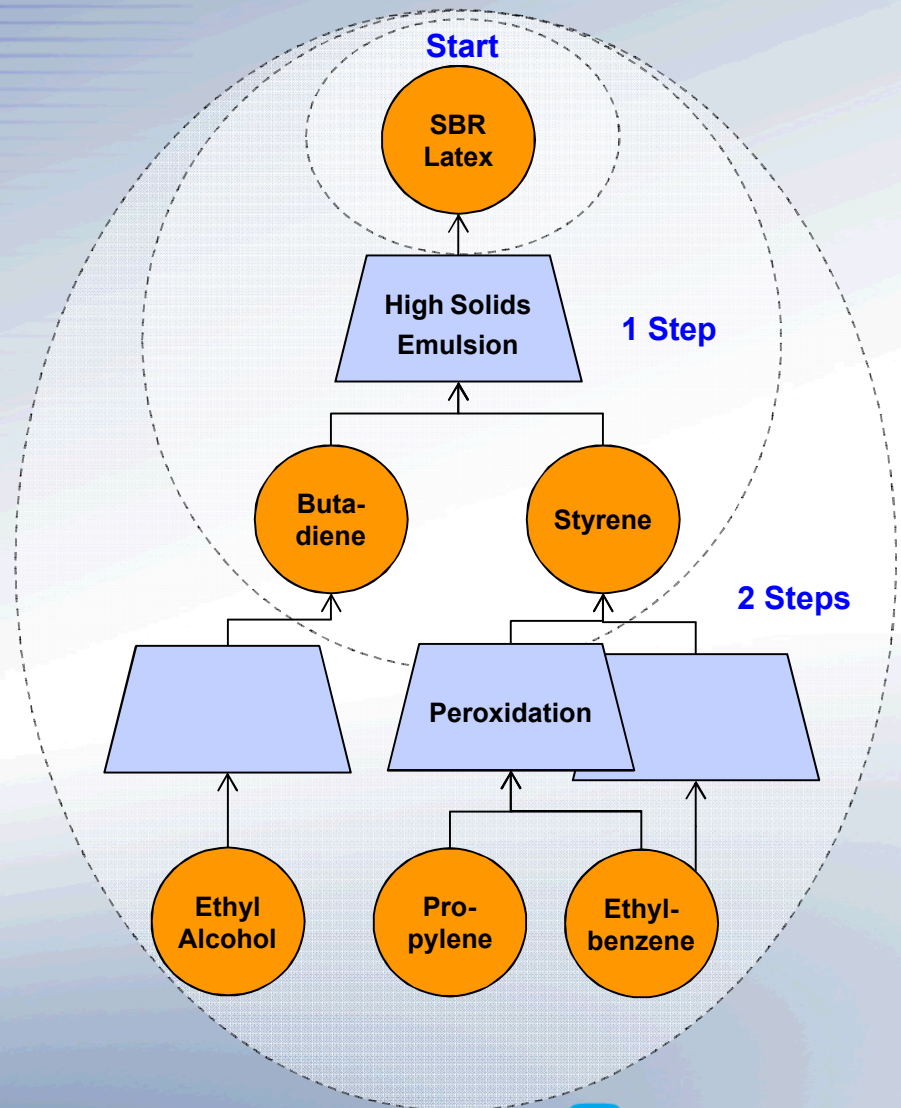
Process Graph Traversal

■ Input:

- Starting chemicals
- # of Steps

■ Output:

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



Model Builder

Builder Configuration File

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

```
<modelbuilder-ocnfig>
```

```
<!-- =====  
  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

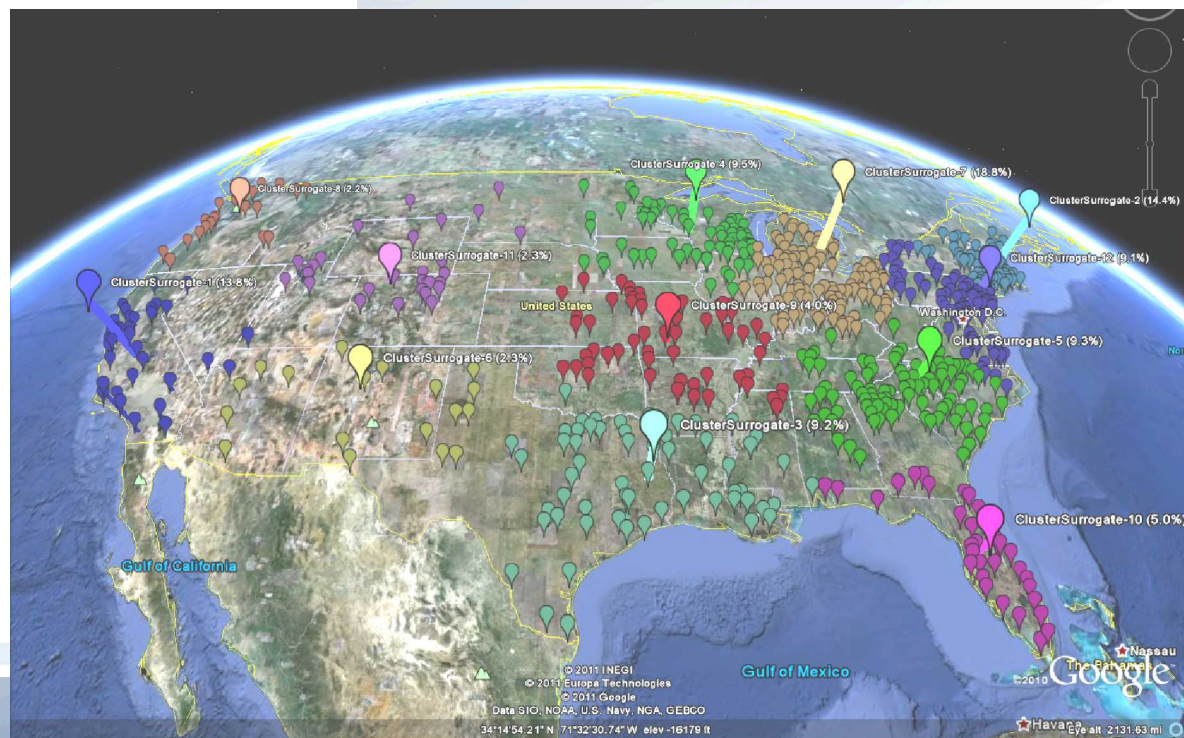
```
<!-- =====  
  TRANSPORTATION  
===== -->
```

Network or simpler 'straight line' shipping

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

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

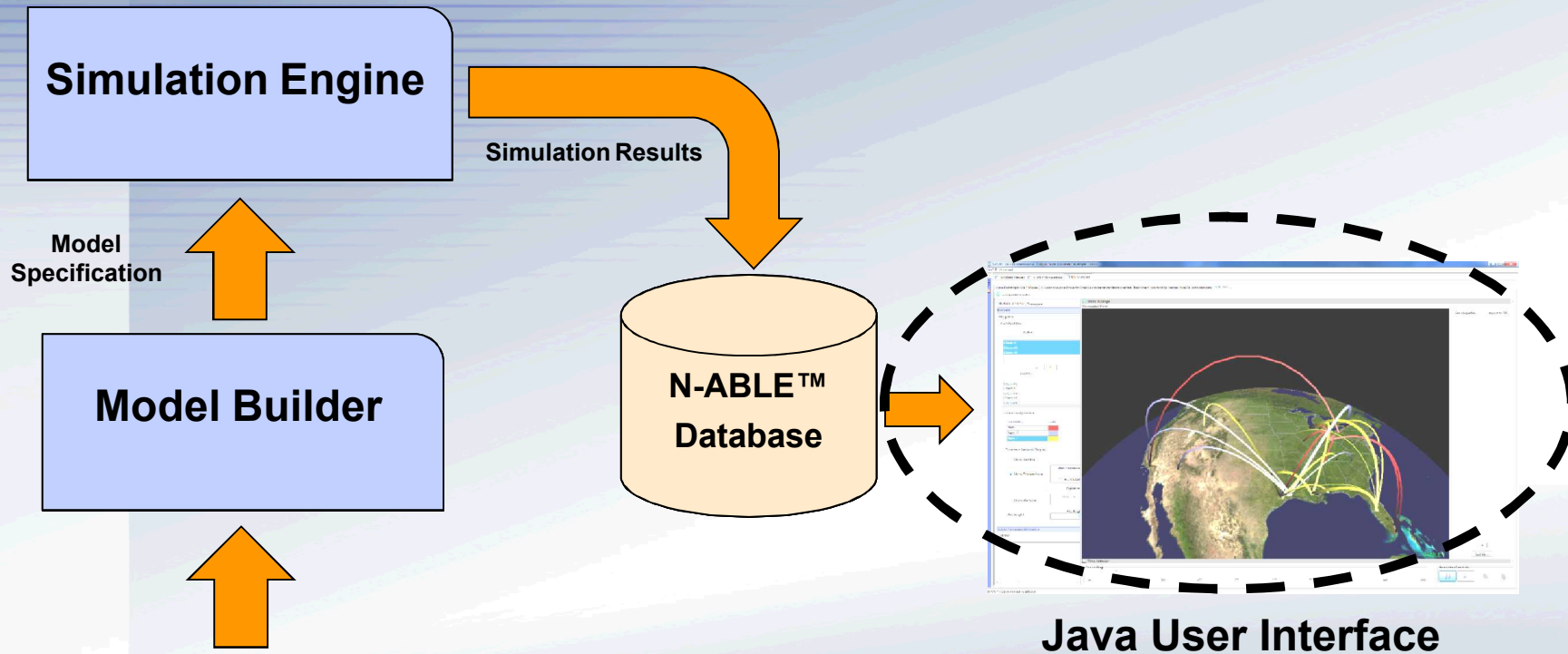
Chemical Demand, Spatial Clustering



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Section: User Interface



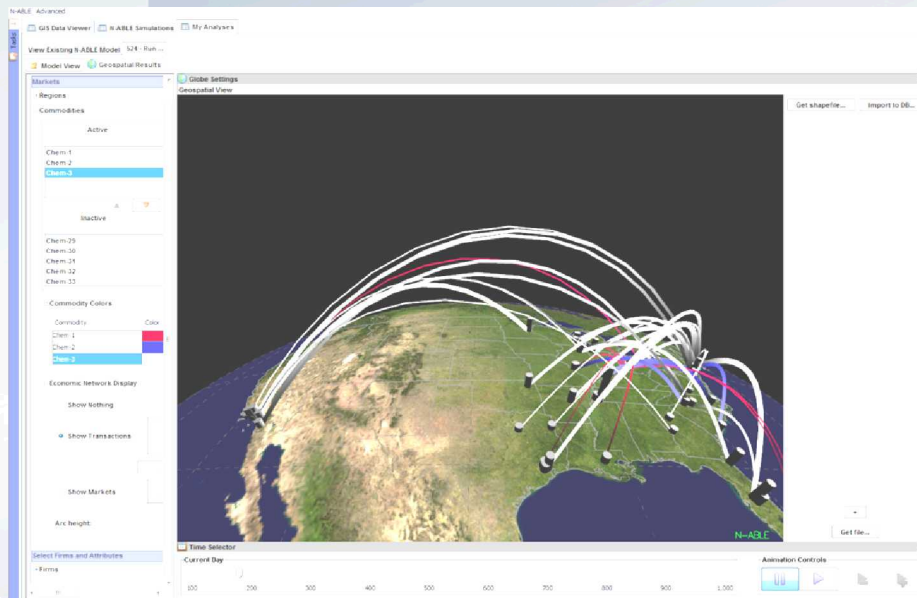
User Interface

■ 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



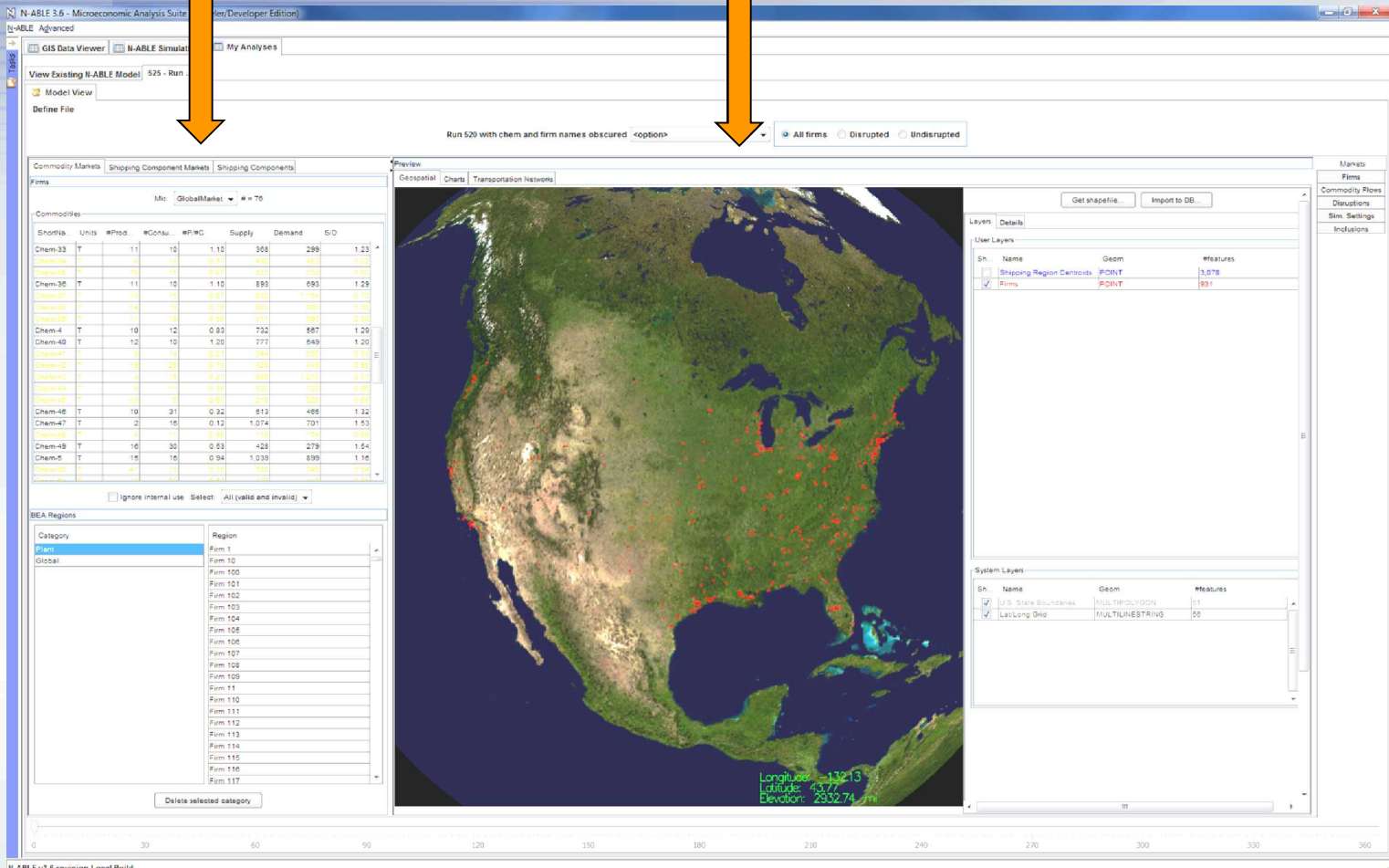
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User Interface: Pre-Simulation

Overall Market Statistics

Geospatial Agent View

Markets Tab



N-ABLE v3.6 revision Local Build

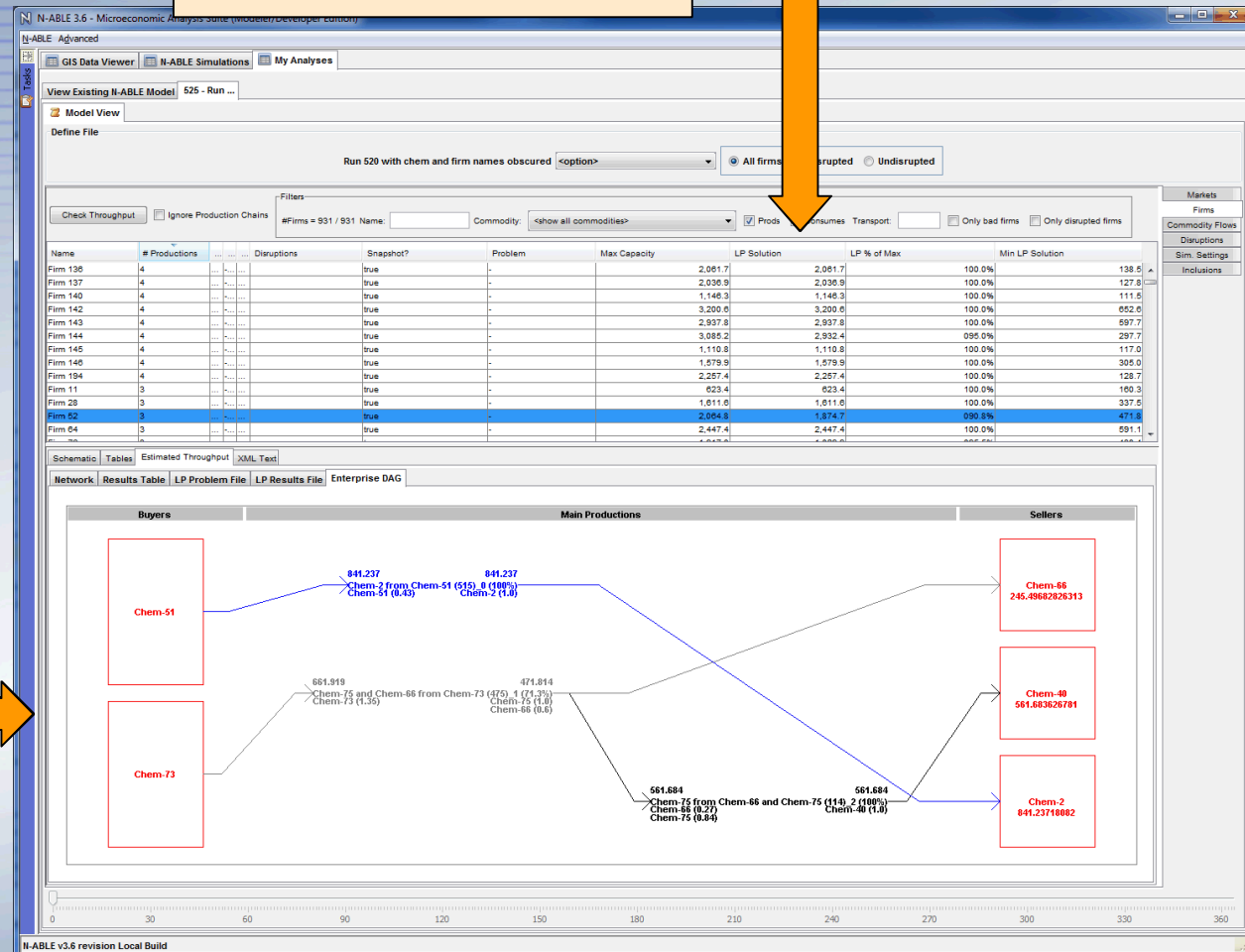
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User Interface: Pre-Simulation

Plant Production
Process Checks

Firms Tab

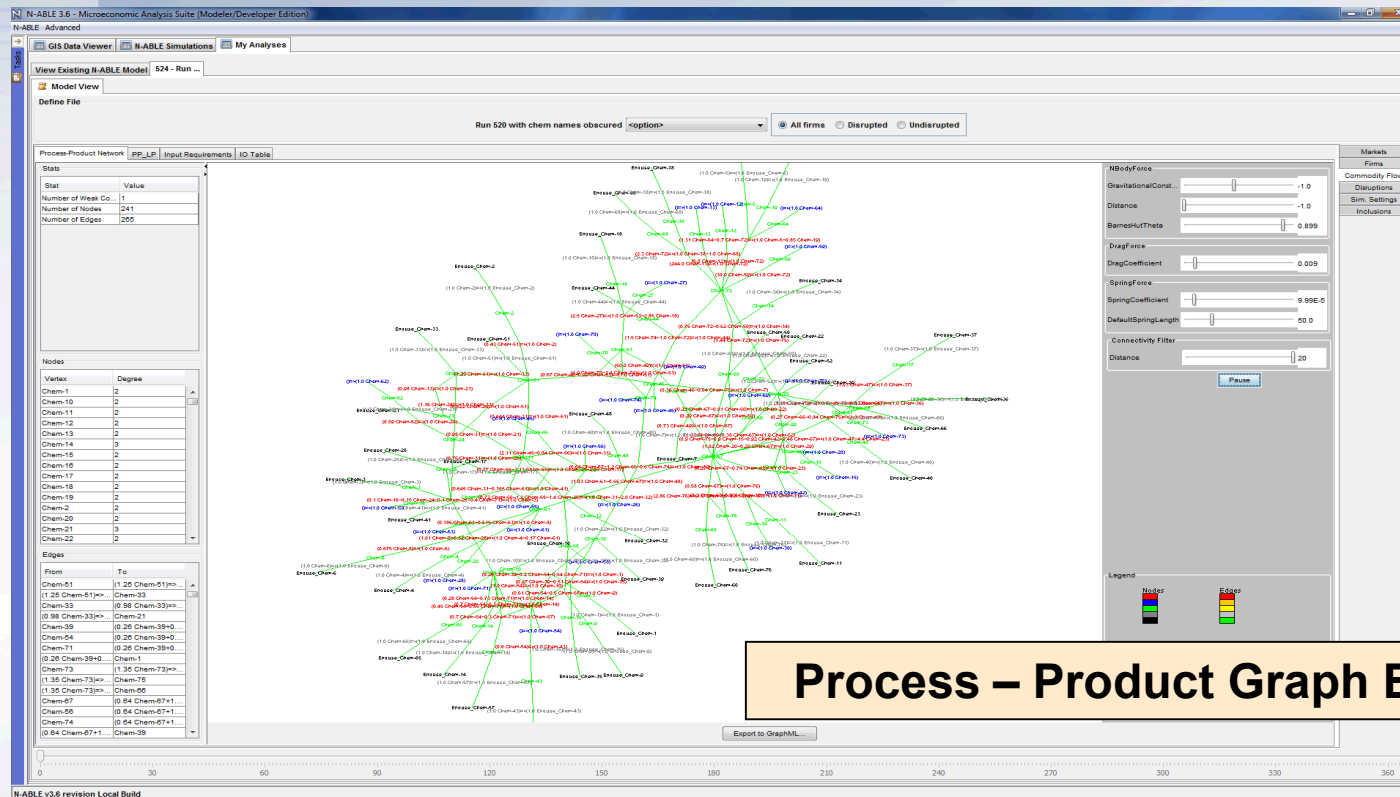
Production
Diagrams



User Interface: Pre-Simulation

End-to-end throughput checks

Commodity Flows Tab



Process – Product Graph Exploration

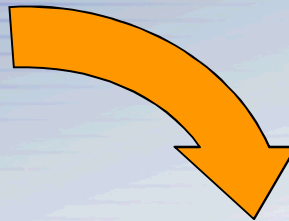
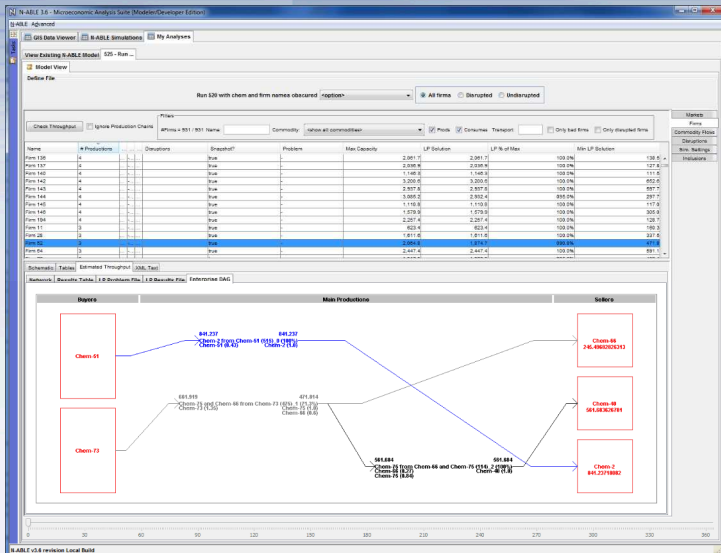


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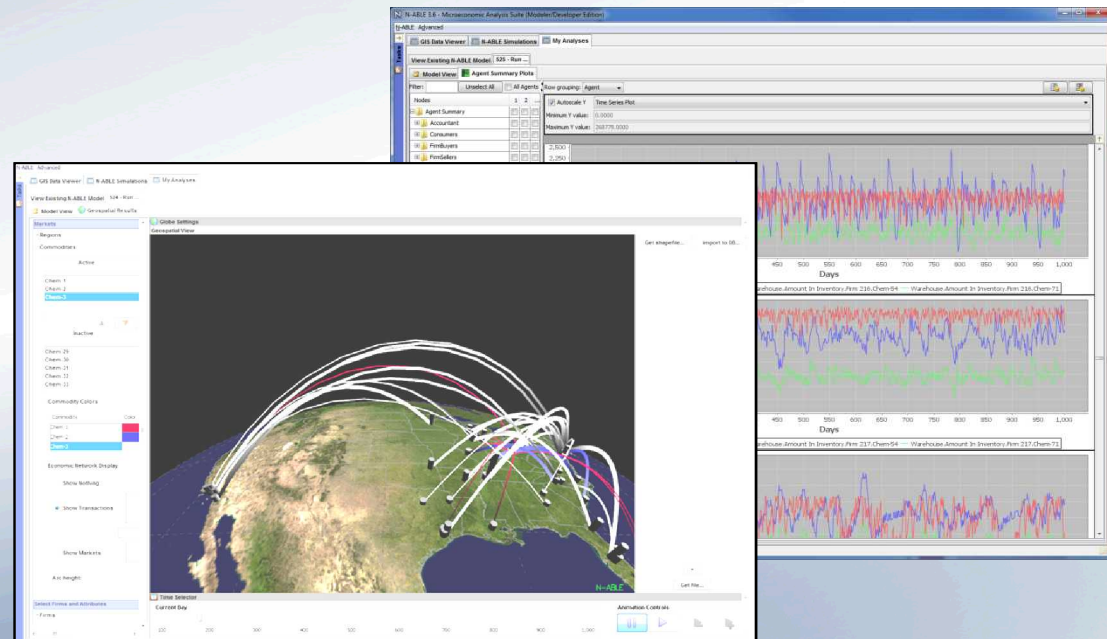


User Interface

Pre-Simulation Analysis



Post-Simulation Analysis



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User Interface: Simulation Archive

Centralized Archive of all Simulations in Database

All inputs are versioned and recorded – traceable and repeatable

Simulations can be promoted to “Baseline” status

Baseline simulations can have disruptions applied

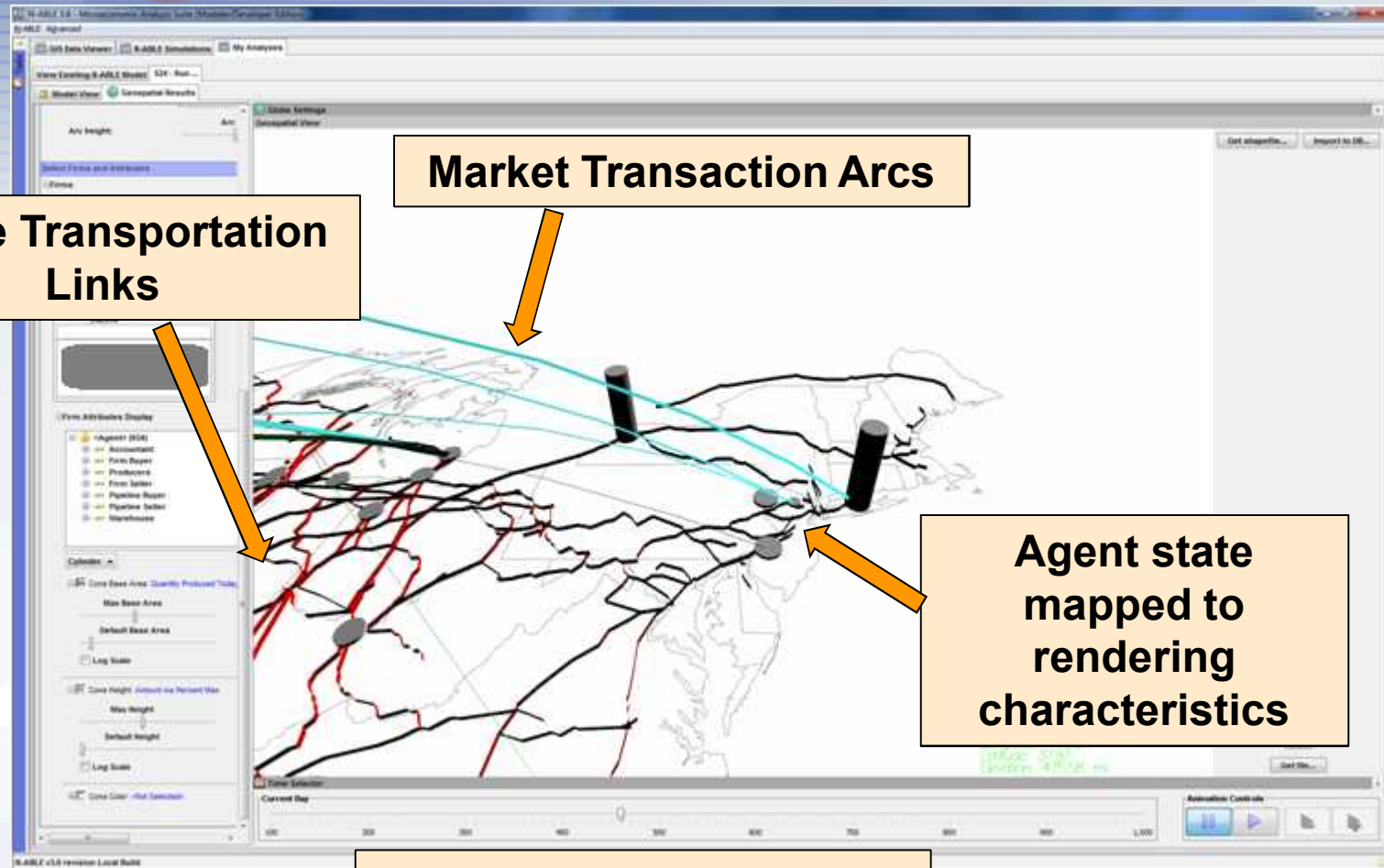
Nodes	Node ID	Owner	Description	Submit Time	% Upload	Engine Ver.
gov.sandia.nable.unitTests.Test_Lp1_Producer	284	<testing>	Testing only -single producer produces until warehou...	Jun 7, 2011 17:...	100.0	1296
gov.sandia.nable.unitTests.Test_Lp2_TwoIndependentConsumer	285	<testing>	Testing only -two 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

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



User Interface: Post-Simulation

Geospatial Simulation Animation



User Interface: Post-Simulation

Time Series Visualization - Aggregates

Data Export

Data Selector

Row =
Commodity



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User Interface: Post-Simulation

Time Series Visualization – Agent Level



User Interface: Disruption Specification

Damage Contour Library

Contour + Agent Viz

The screenshot displays a software interface for specifying disruptions. It is divided into three main panels:

- Damage Contour Library:** Located on the left, it contains two sections: "Available Contours" and "Model Disruptions".
 - Available Contours:** A list of contour names. The selected item is "dmg_nmsz_day1_3_ep_outage_100_wgs84".
 - Model Disruptions:** A table showing the configuration of model disruptions.
- Scenario Specification:** Located at the bottom left, it contains a "Run Simulation" button and a "Delete all" button.
- Contour + Agent Viz:** The central map panel showing a satellite view of the United States with red dots representing agents and orange concentric circles representing damage contours. A status bar at the bottom right of the map displays: Longitude: -80.48, Latitude: 29.41, Elevation: 2140.11 mi.

On the right side of the interface, there is a "Layers" panel with two tabs: "User Layers" and "System Layers".

User Layers:

Sh...	Name	Geom
<input checked="" type="checkbox"/>	chemical_plant_damag...	MULTIPOLYGON
<input checked="" type="checkbox"/>	dmg_nmsz_day1_3_ep...	MULTIPOLYGON
<input checked="" type="checkbox"/>	dmg_nmsz_day1_3_ep...	MULTIPOLYGON
<input checked="" type="checkbox"/>	Firms	POINT

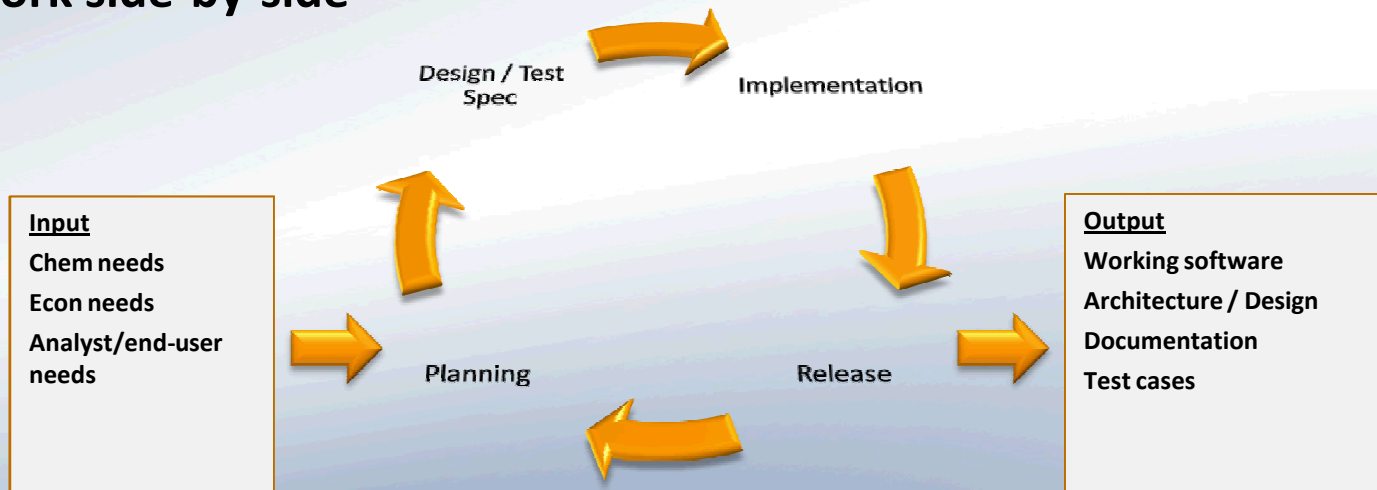
System Layers:

Sh...	Name	Geom
<input checked="" type="checkbox"/>	Lat/Long Grid	MULTILINESTRING
<input checked="" type="checkbox"/>	U.S. State Boundaries	MULTIPOLYGON



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

The screenshot displays the TeamForge web interface for Sandia National Laboratories. The top navigation bar includes links for Projects, My Workspace, Search, History, SNL Support Project, and openCollabNet. The user is logged in as Brian Jones (bsjone). The main project is N-ABLE, with a search bar for artifacts. The left sidebar shows a tree view of Planning Folders, including N-ABLE 3.3, N-ABLE 3.4, and N-ABLE 3.5 (selected). The main content area shows the 'List Artifacts' view for N-ABLE 3.5. It includes a summary section with fields for Name, Description, Effort, Story Points, Start Date, End Date, and File Release. A Burndown chart and a pie chart showing Open (0) and Closed (42) artifacts are also present. Below the summary is a table of artifacts with columns for Priority, Artifact ID, Title, Assigned To, Status, and Planned For.

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



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

