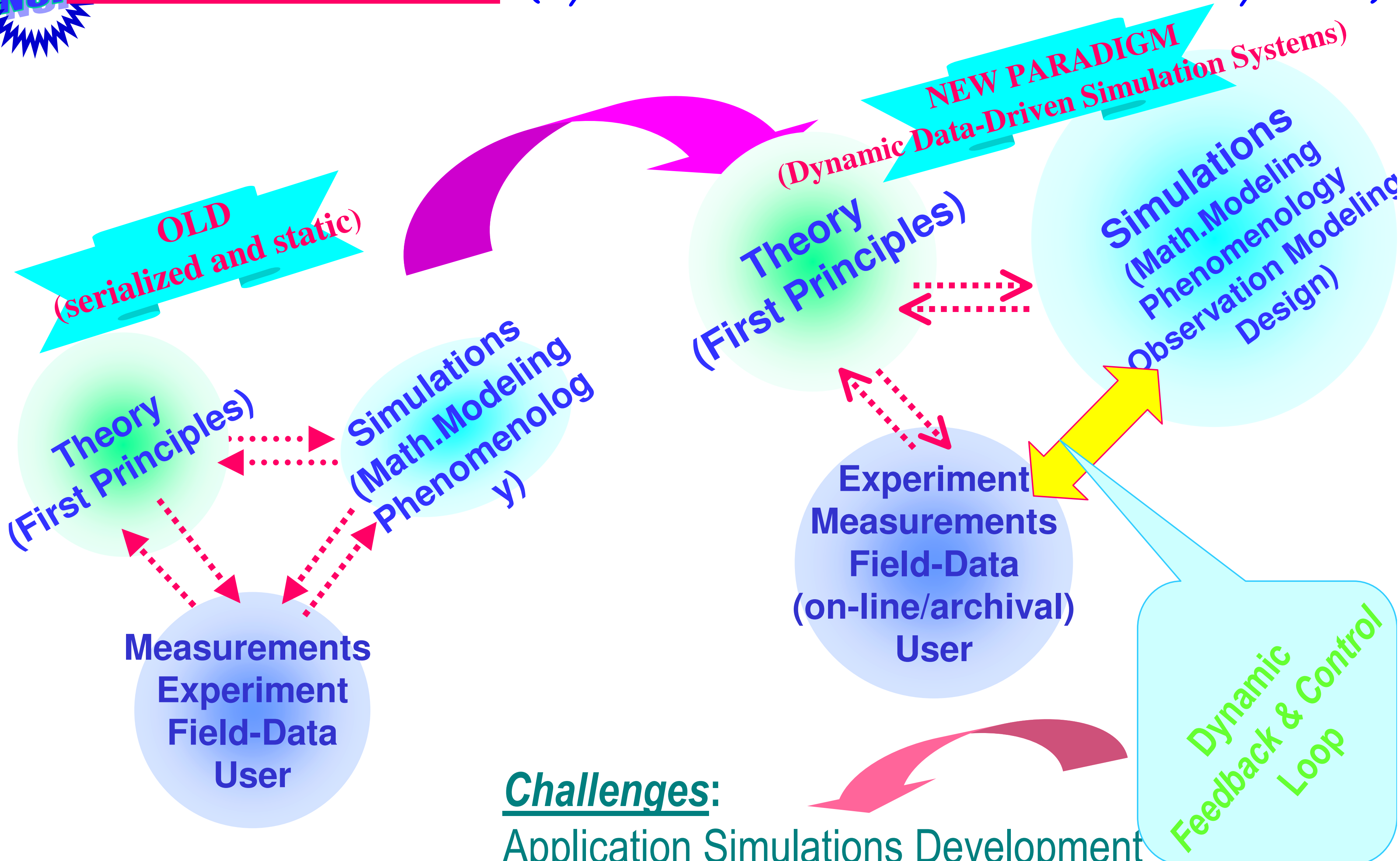
Dynamic Data Driven Application Systems (DDDAS)

A new paradigm for applications/simulations <u>and</u> measurement methodology

and why systems software is important here, …and how it would impact CyberInfrastructure!

Dr. Frederica Darema
Senior Science and Technology Advisor
Director, Next Generation Software Program
NSF

What is DDAS (*Symbiotic Measurement&Simulation Systems*)



Challenges:

Application Simulations Development

Algorithms

Computing Systems Support

Examples of Applications benefiting from the new paradigm

- Engineering (Design and Control)
  - aircraft design, oil exploration, semiconductor mfg, structural eng
  - computing systems hardware and software design
    (performance engineering)
- Crisis Management and Environmental Systems
  - transportation systems (planning, accident response)
  - weather, hurricanes/tornadoes, floods, fire propagation
- Medical
  - customized surgery, radiation treatment, etc
  - BioMechanics /BioEngineering
- Manufacturing/Business/Finance
  - Supply Chain (Production Planning and Control)
  - Financial Trading (Stock Mkt, Portfolio Analysis)

DDDAS has the potential to revolutionize science, engineering, & management systems

NSF March 2000 Workshop on DDAS

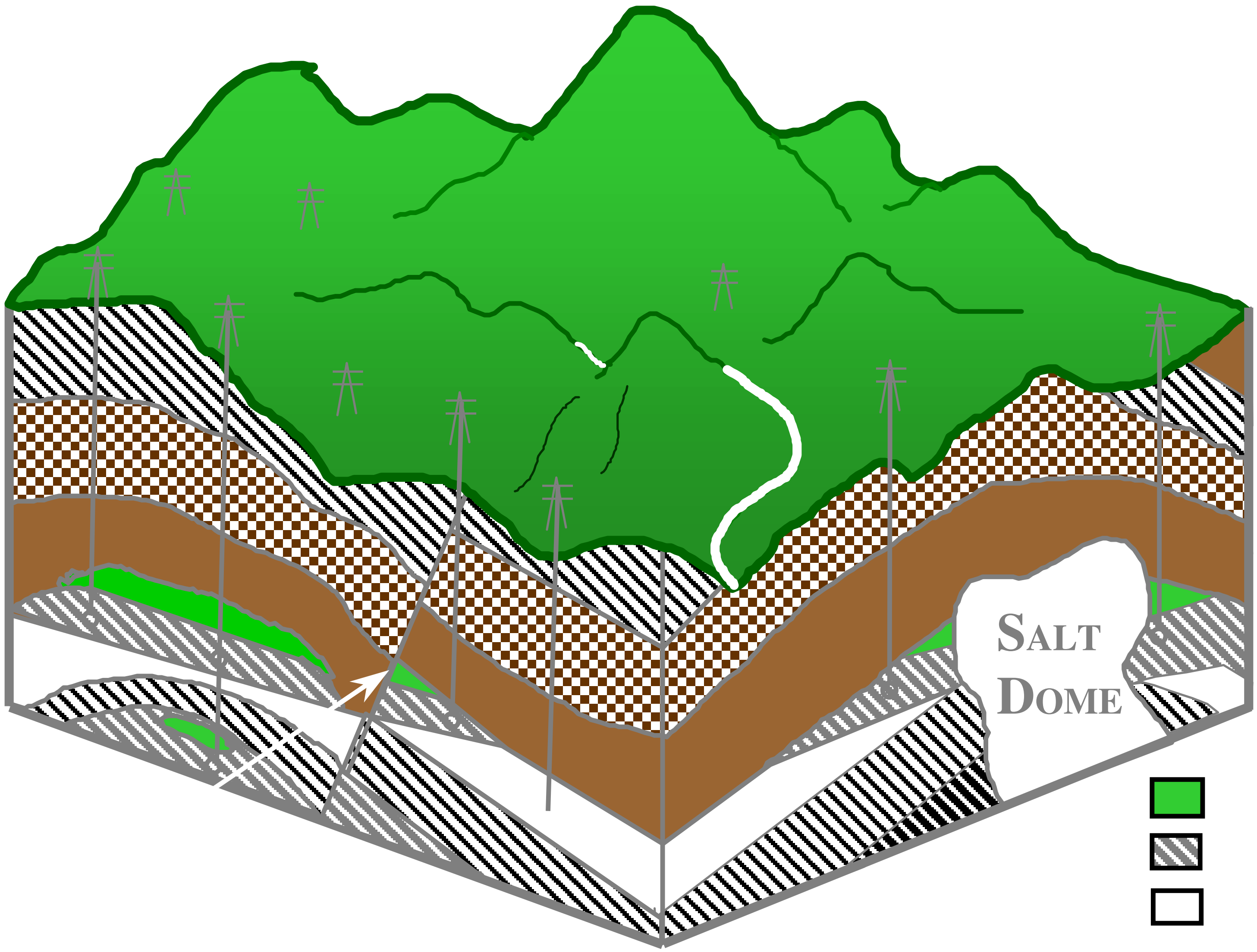
(Co-Chairs: Craig Douglas, UKy; Abhi Desmukh, UMass)

Invited Presentations

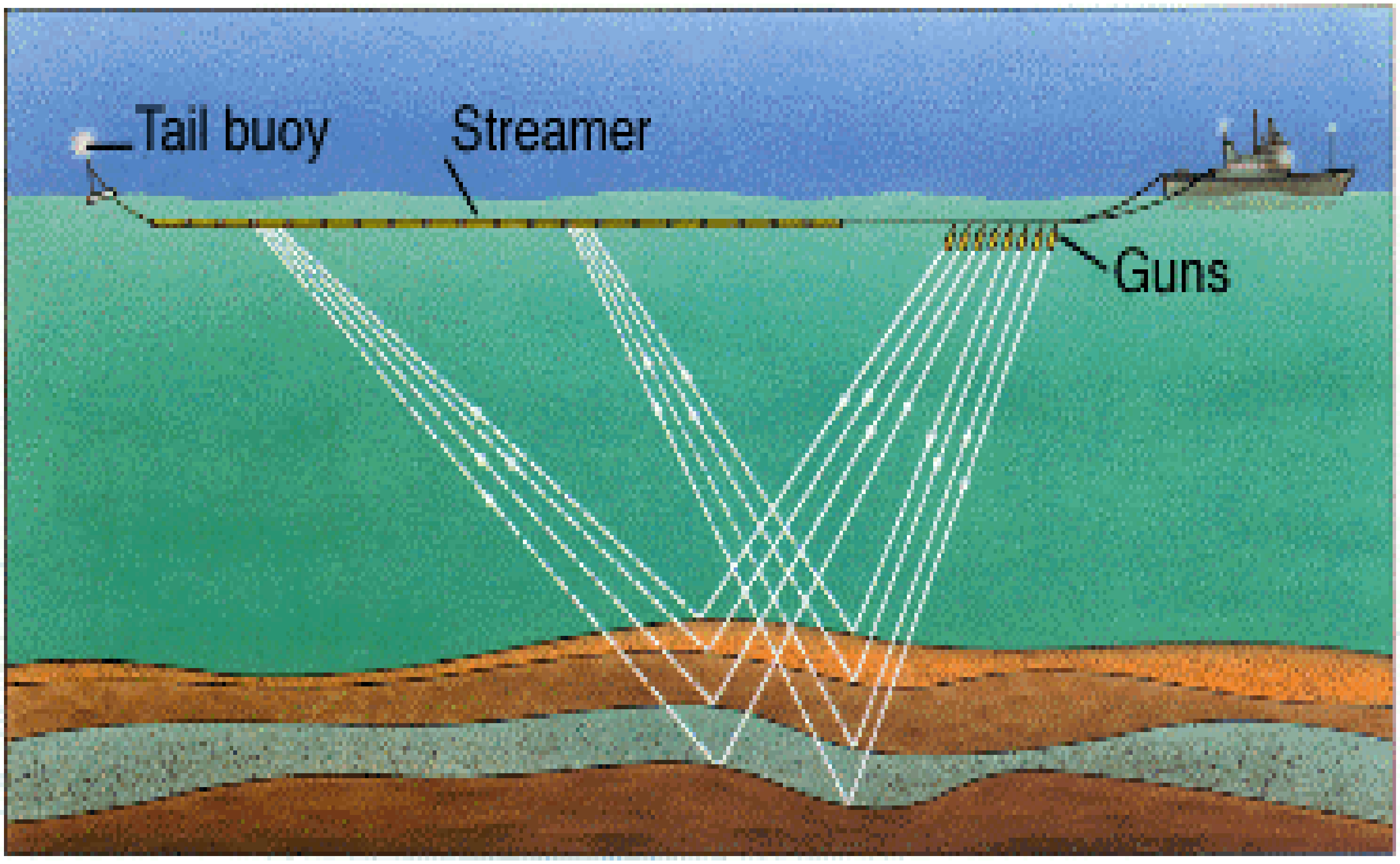
- New Directions on Model-Based Data Assimilation (Chemical Appl's)
  Greg McRae, Professor, MIT
- Coupled atmosphere-wildfire modeling
  Janice Coen, Scientist, NCAR
- Data/Analysis Challenges in the Electronic Commerce Environment
  Howard Frank, Dean, Business School, UMD
- Steered computing - A powerful new tool for molecular biology
  Klaus Schulten, Professor, UIUC, Beckman Institute
- Interactive Control of Large-Scale Simulations
  Dick Ewing, Professor, Texas A&M University
- Interactive Simulation and Visualization in Medicine: Applications to Cardiology, Neuroscience and Medical Imaging
  Chris Johnson, Professor, University of Utah
- Injecting Simulations into Real Life
  Anita Jones, Professor, UVA

Workshop Report: www.cise.nsf.gov/dddas

PETROLEUM APPLICATIONS

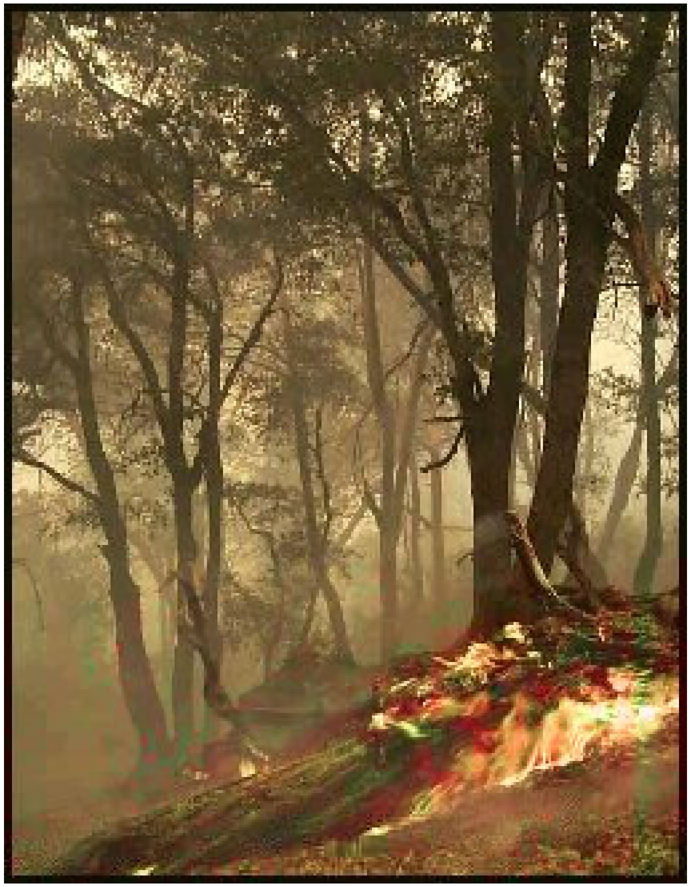


Surface hydrophone array



Fire Model

- Sensible and latent heat fluxes from ground and canopy fire -> heat fluxes in the atmospheric model.
- Fire's heat fluxes are absorbed by air over a specified extinction depth.
- 56% fuel mass -> H_2O vapor
- 3% of sensible heat used to dry ground fuel.
- Ground heat flux used to dry and ignite the canopy.



Kirk Complex Fire. U.S.F.S. photo

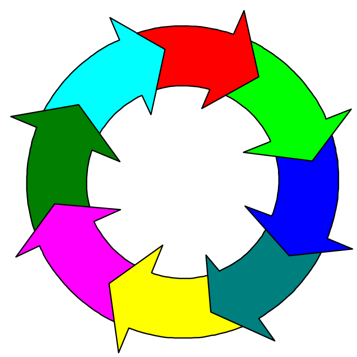
Slide Courtesy of Coen/NCAR

Coupled atmospheric and wildfire models

FIRE

ATMOSPHERE

Sensible and Latent Heat

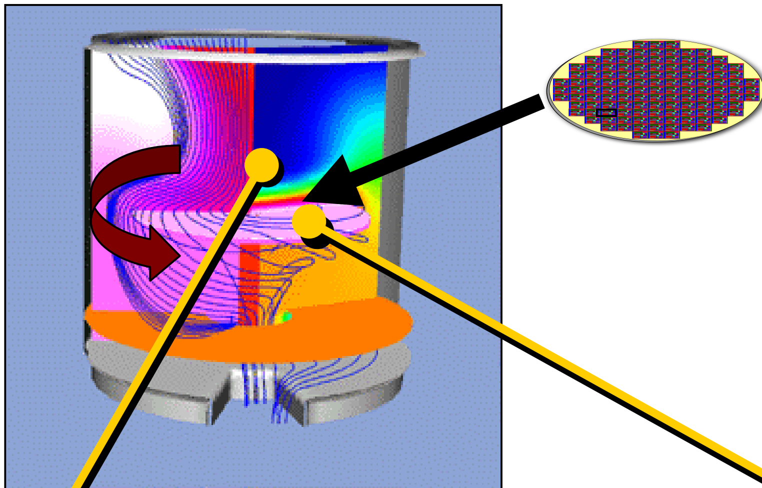


Atmospheric Dynamics

Fire Propagation

Slide Courtesy of Coen/NCAR

AMAT Centura Chemical Vapor Deposition Reactor



Operating Conditions

Reactor Pressure	1 atm
Inlet Gas Temperature	698 K
Surface Temperature	1173 K
Inlet Gas-Phase Velocity	46.6 cm/sec

Gas Phase Reactions

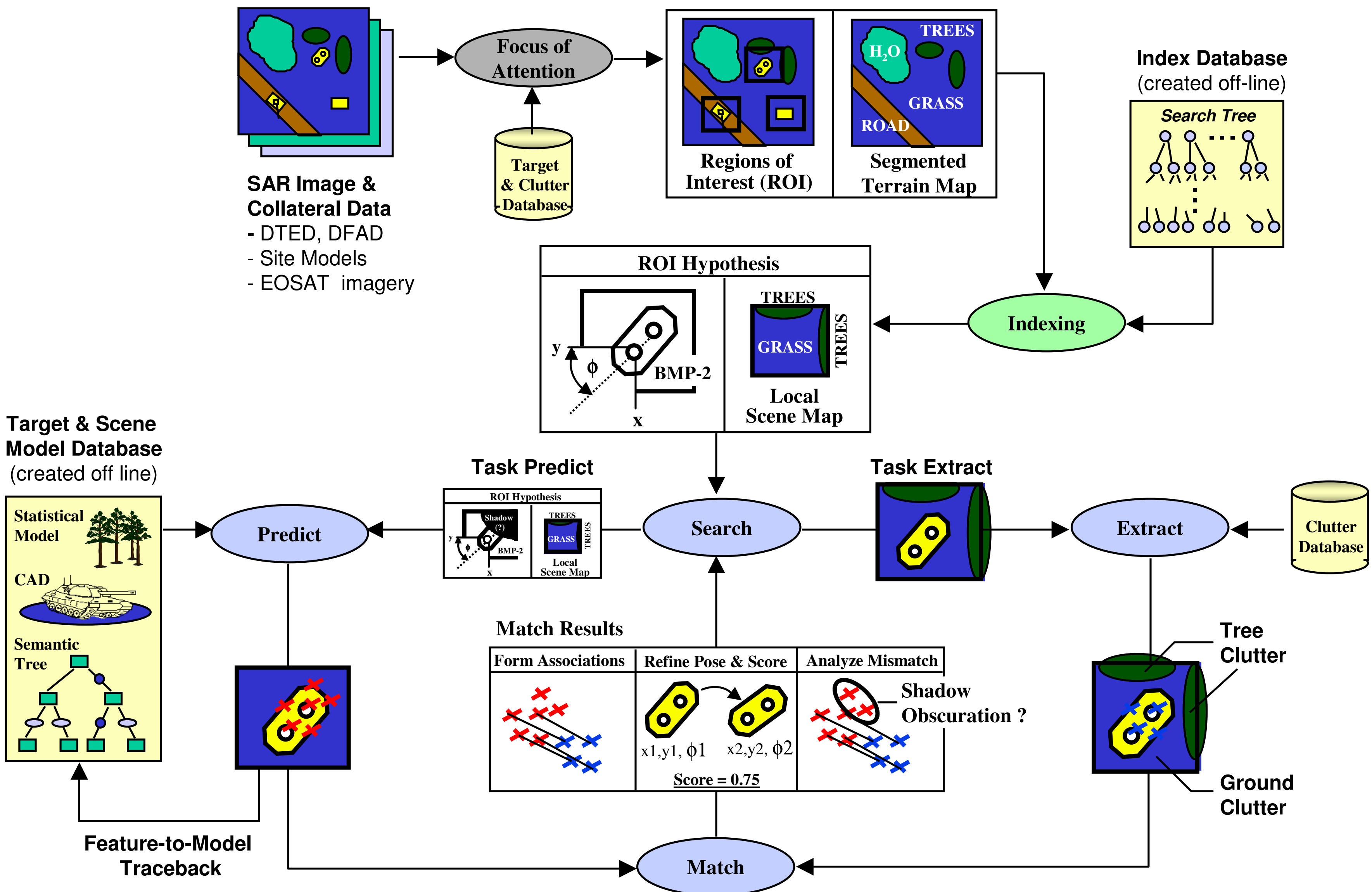
$SiCl_3H \Rightarrow HCl + SiCl_2$
$SiCl_2H_2 \Rightarrow SiCl_2 + H_2$
$SiCl_2H_2 \Rightarrow HSiCl + HCl$
$H_2ClSiSiCl_3 \Rightarrow SiCl_4 + SiH_2$
$H_2ClSiSiCl_3 \Rightarrow SiCl_3H + HSiCl$
$H_2ClSiSiCl_3 \Rightarrow SiCl_2H_2 + SiCl_2$
$Si_2Cl_5H \Rightarrow SiCl_4 + HSiCl$
$Si_2Cl_5H \Rightarrow SiCl_3H + SiCl_2$
$Si_2Cl_6 \Rightarrow SiCl_4 + SiCl_2$

Surface Reactions

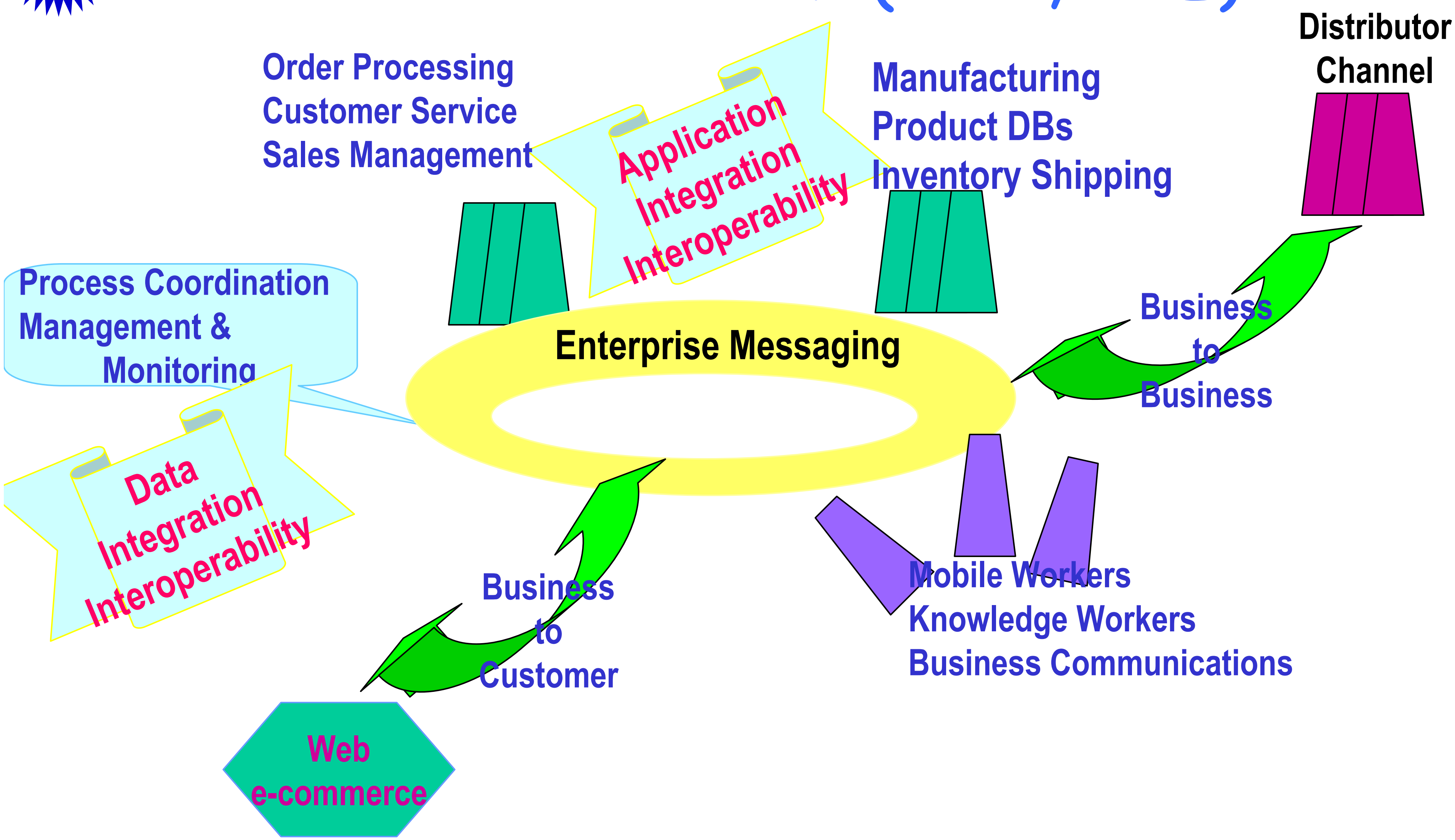
$SiCl_3H + 4s \Rightarrow Si(B) + sH + 3sCl$
$SiCl_2H_2 + 4s \Rightarrow Si(B) + 2sH + 2sCl$
$SiCl_4 + 4s \Rightarrow Si(B) + 4sCl$
$HSiCl + 2s \Rightarrow Si(B) + sH + sCl$
$SiCl_2 + 2s \Rightarrow Si(B) + 2sCl$
$2sCl + Si(B) \Rightarrow SiCl_2 + 2s$
$H_2 + 2s \Rightarrow 2sH$
$2sH \Rightarrow 2s + H_2$
$HCl + 2s \Rightarrow sH + sCl$
$sH + sCl \Rightarrow 2s + HCl$

Slide Courtesy of McRae/MIT

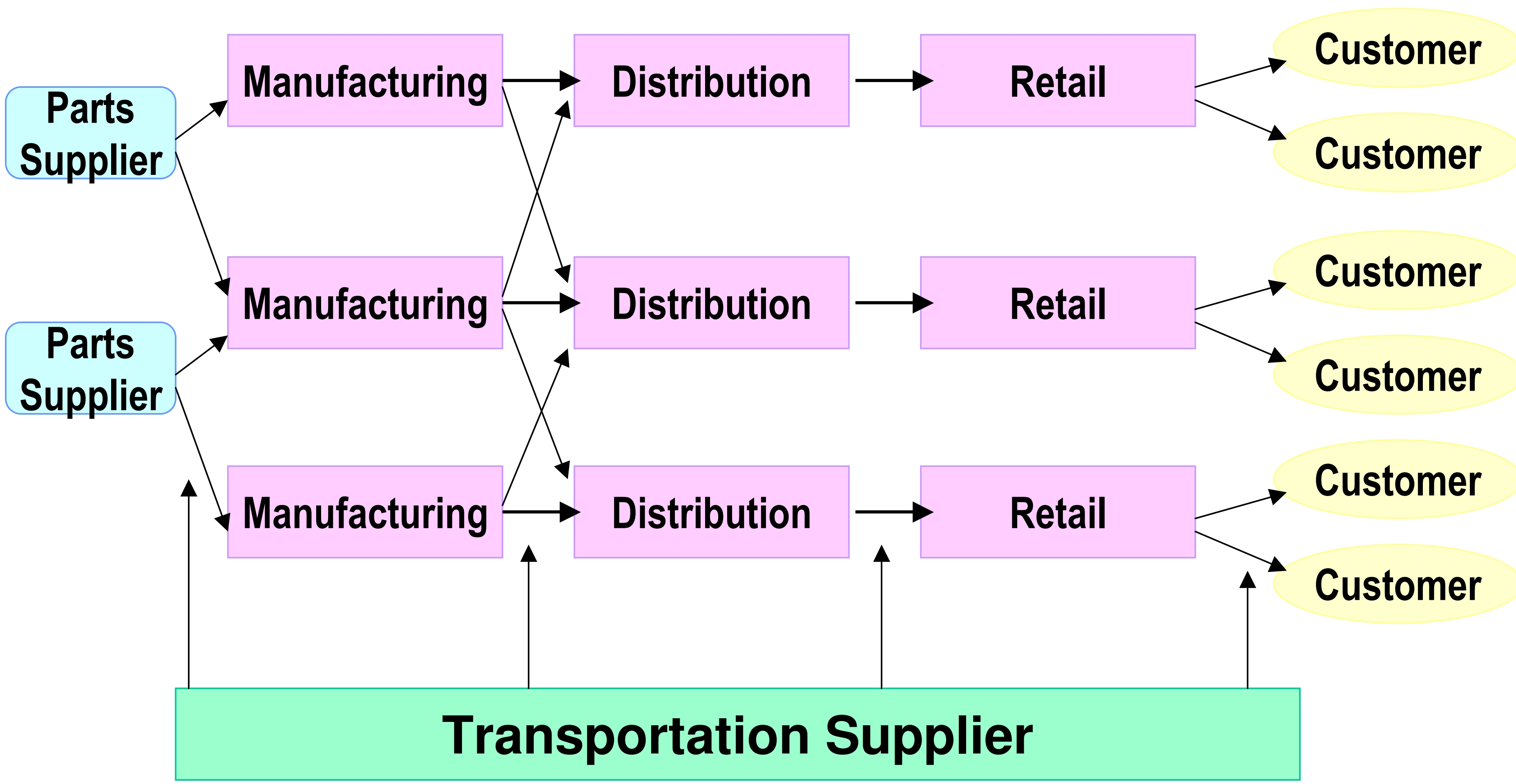
MSTAR (DARPA)
(Moving and Stationary Target Acquisition and Recognition)



The e-Business / (CIM, CIE)



Compare with
Classical (Old) Supply Chain

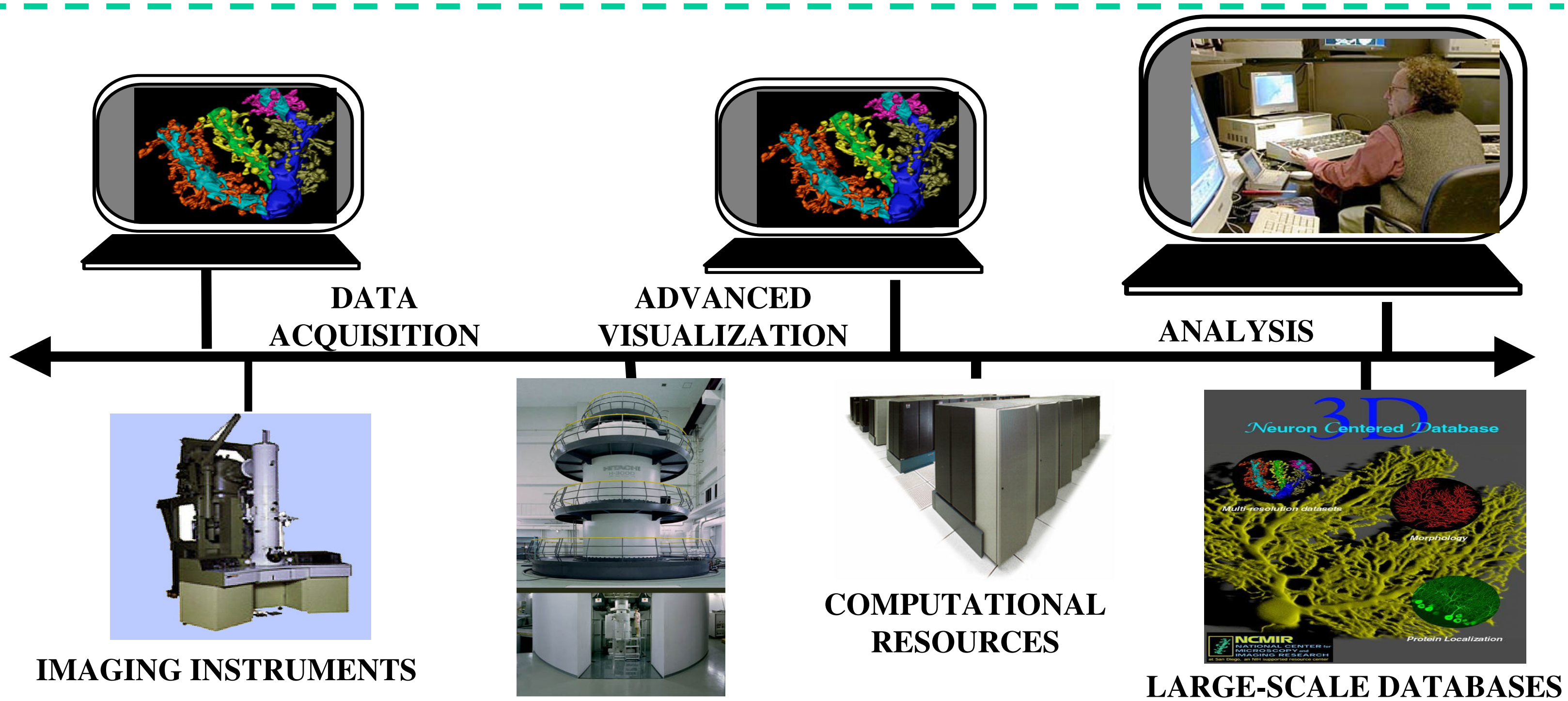


Some Technology Challenges in Enabling DDAS

- **Application development**
  - interfaces of applications with measurement systems
  - dynamically select appropriate application components
  - ability to switch to different algorithms/components depending on streamed data
- **Algorithms**
  - tolerant to perturbations of dynamic input data
  - handling data uncertainties
- **Systems supporting such dynamic environments**
  - dynamic execution support on heterogeneous environments
  - Extended Spectrum of platforms: assemblies of Sensor Networks and Computational Grid platforms
  - GRID Computing, and Beyond!!!

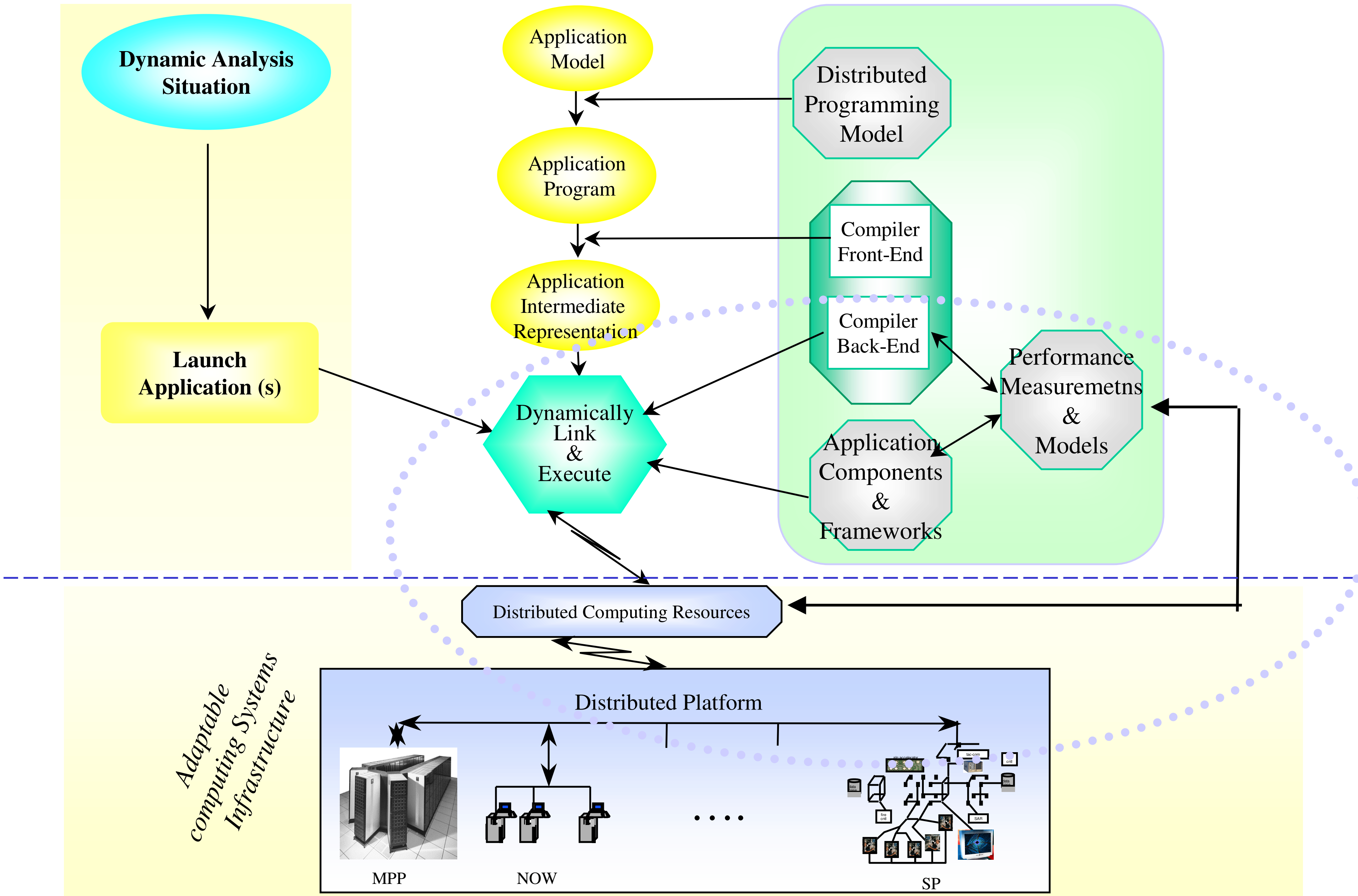
What is Grid Computing?

coordinated problem solving on dynamic and heterogeneous resource assemblies



Example: "Telescience Grid", Courtesy of Ellisman & Berman /UCSD&NPACI

The NGS Program develops Technology for integrated feedback & control
Runtime Compiling System (RCS) and Dynamic Application Composition



Some more Challenges on Applications Development Issues

- Handling Data Streams in addition to Data Sets
- Handling different data structures – semantic information
- Interfaces to Measurement Systems
  - Interactive Visualization and Steering
- Standards for data exchange
- Combining Local and Global Knowledge
- Model Interactions
- Application control of measurement systems
- Dynamic Application Composition and Runtime support

(Examples from ITR supported efforts)

Important Point:

DDDAS is not just DATA ASSIMILATION!!!

- Data Assimilation compares/corrects specific calculated points with experiments, rather than dynamically as need
- Data Assimilation does not include the notion of the simulation/application controlling the measurement process

Rather…

Data Assimilation techniques can be used in certain DDDAS cases

Programming Environments

- Procedural - > Model Based
- Programming -> Composition
- Custom Structures -> Customizable Structures (patterns, templates)
- Libraries -> Frameworks -> Compositional Systems (*Knowledge Based Systems*)
- Application Composition Frameworks

and....

- Interoperability extended to include measurements
- Data Models and Data Management
  - Extend the notion of Data Exchange Standards (Applications and Measurements)

Additional Considerations/Requirements on Hardware and Software Systems

- Extended Spectrum of platforms
  - Assemblies of Computational Grid and Sensor Networks platforms
- Systems Architectures including Measurement Systems
- Programming Environments
- Application, System, and Resource Management
- Models of the Computational Infrastructure
- Security and Fault Tolerance
- DDDAS will accentuate and create the need for advances in such areas

Towards
Enabling DDDAS

Today's Grid Environments:
"Users shouldn't Have to be Heroes
to Achieve Grid Program Performance"
and… because heroism is not enough

Impact to CyberInfrastructure

- The CyberInfrastructure that will result when thinks of the present paradigm of (disjoint) simulations and measurements will be different than the CyberInfrastructure needed to support DDDAS
- For example, bandwidth requirements, resource allocation and other middleware and systems software policies, prioritization, security, fault tolerance, recovery, QoS, etc…, will be different when one needs to guarantee data streaming to an executing simulation or control of measurement process

Why Now is the Time for DDAS

- Technological progress has prompted advances in some of the challenges
  - Computing speeds advances (uni- and multi-processor systems), Grid Computing, Sensor Networks
  - Systems Software
  - Applications Advances (parallel & grid computing)
  - Algorithms advances (parallel &grid computing, numeric and non-numeric techniques: dynamic meshing, data assimilation)
- Examples of efforts in:
  - Systems Software
  - Applications
  - Algorithms

Agency Efforts

NSF

- NGS: The Next Generation Software Program (1998-)
  - develops systems software supporting dynamic resource execution
- Scalable Enterprise Systems Program (1999, 2000-2003)
  - geared towards "commercial" applications (Chaturvedi example)
- ITR: Information Technology Research (**NSF-wide, FY00-04**)
  - has been used as an opportunity to support DDDAS related efforts
  - In FY00 1 NGS/DDDAS proposal received; deemed best, funded
  - In FY01, 46 ~DDDAS pre-proposals received; many meritorious; 24 proposals received; 8 were awarded
  - In FY02, 31 ~DDDAS proposals received; 8(10) awards
  - In FY02, so far: received 35 ("Small" ITR) proposals ~DDDAS; more expected in the "Medium ITR" category -
- Gearing towards a DDDAS program
  - expect participation from other NSF Directorates
  - *Looking for participation from other agencies!*

"~DDDAS" proposals awarded in FY00 ITR Competition

- **Pingali, Adaptive Software for Field-Driven Simulations**

"~DDDAS" proposals awarded in FY01 ITR Competition

- Biegler – Real-Time Optimization for Data Assimilation and Control of Large Scale Dynamic Simulations
- Car – Novel Scalable Simulation Techniques for Chemistry, Materials Science and Biology
- Knight – Data Driven design Optimization in Engineering Using Concurrent Integrated Experiment and Simulation
- Lonsdale – The Low Frequency Array (LOFAR) – A Digital Radio Telescope
- McLaughlin – An Ensemble Approach for Data Assimilation in the Earth Sciences
- Patrikalakis – Poseidon – Rapid Real-Time Interdisciplinary Ocean Forecasting: Adaptive Sampling and Adaptive Modeling in a Distributed Environment
- Pierrehumbert- Flexible Environments for Grand-Challenge Climate Simulation
- Wheeler- Data Intense Challenge: The Instrumented Oil Field of the Future

"~DDDAS" proposals awarded in FY02 ITR Competition

- **Carmichael – Development of a general Computational Framework for the Optimal Integration of Atmospheric Chemical Transport Models and Measurements Using Adjoints**
- **Douglas-Ewing-Johnson – Predictive Contaminant Tracking Using Dynamic Data Driven Application Simulation (DDDAS) Techniques**
- **Evans – A Framework for Environment-Aware Massively Distributed Computing**
- **Farhat – A Data Driven Environment for Multi-physics Applications**
- **Guibas – Representations and Algorithms for Deformable Objects**
- **Karniadakis – Generalized Polynomial Chaos: Parallel Algorithms for Modeling and Propagating Uncertainty in Physical and Biological Systems**
- **Oden – Computational Infrastructure for Reliable Computer Simulations**
- **Trafalis – A Real Time Mining of Integrated Weather Data**

Measured Response

A Homeland Security Simulation

(Briefed WH 5/14/02)

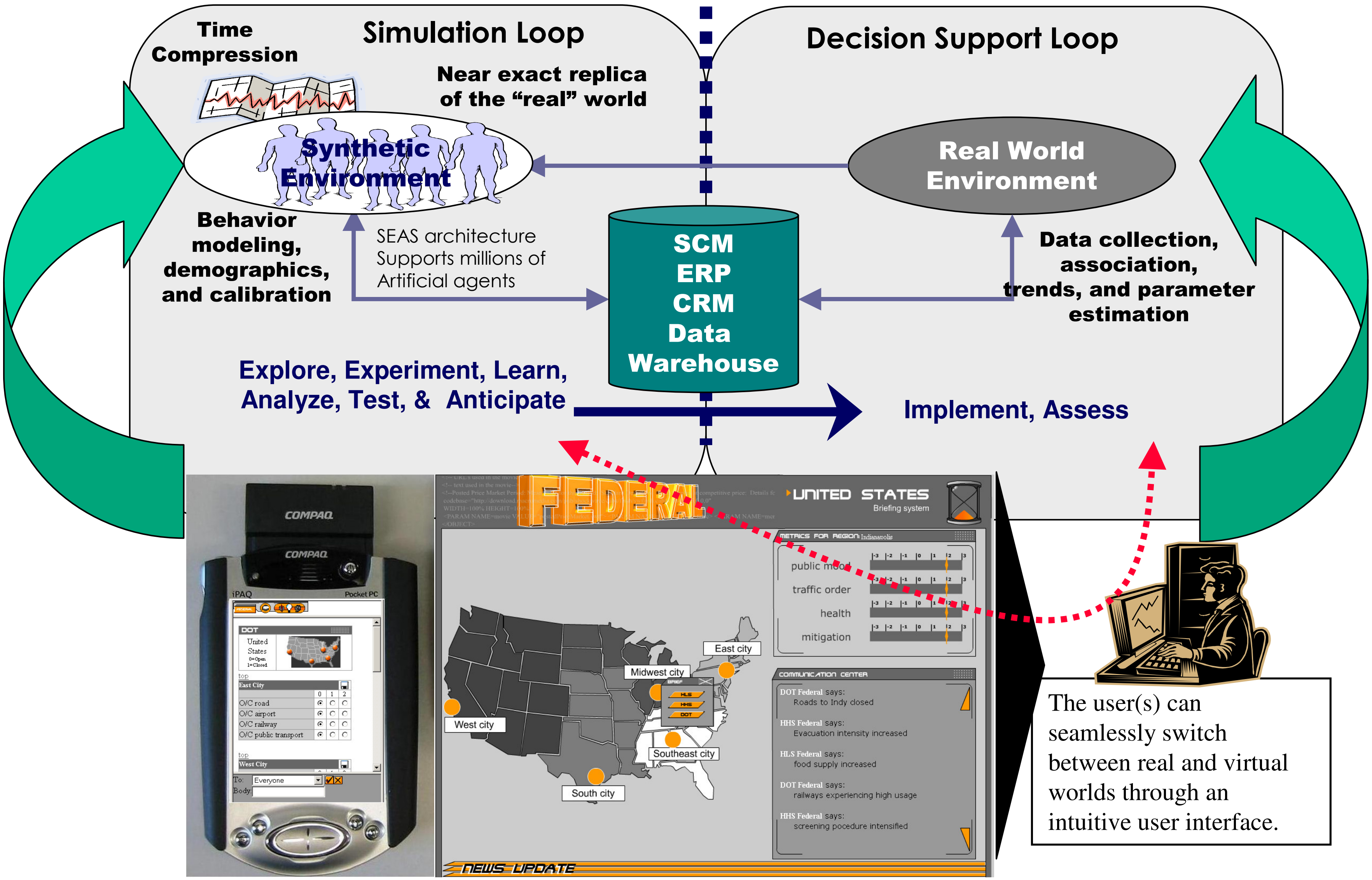
Alok Chaturvedi, Director
Shailendra Mehta, co-Director

Purdue e-Business Research Center

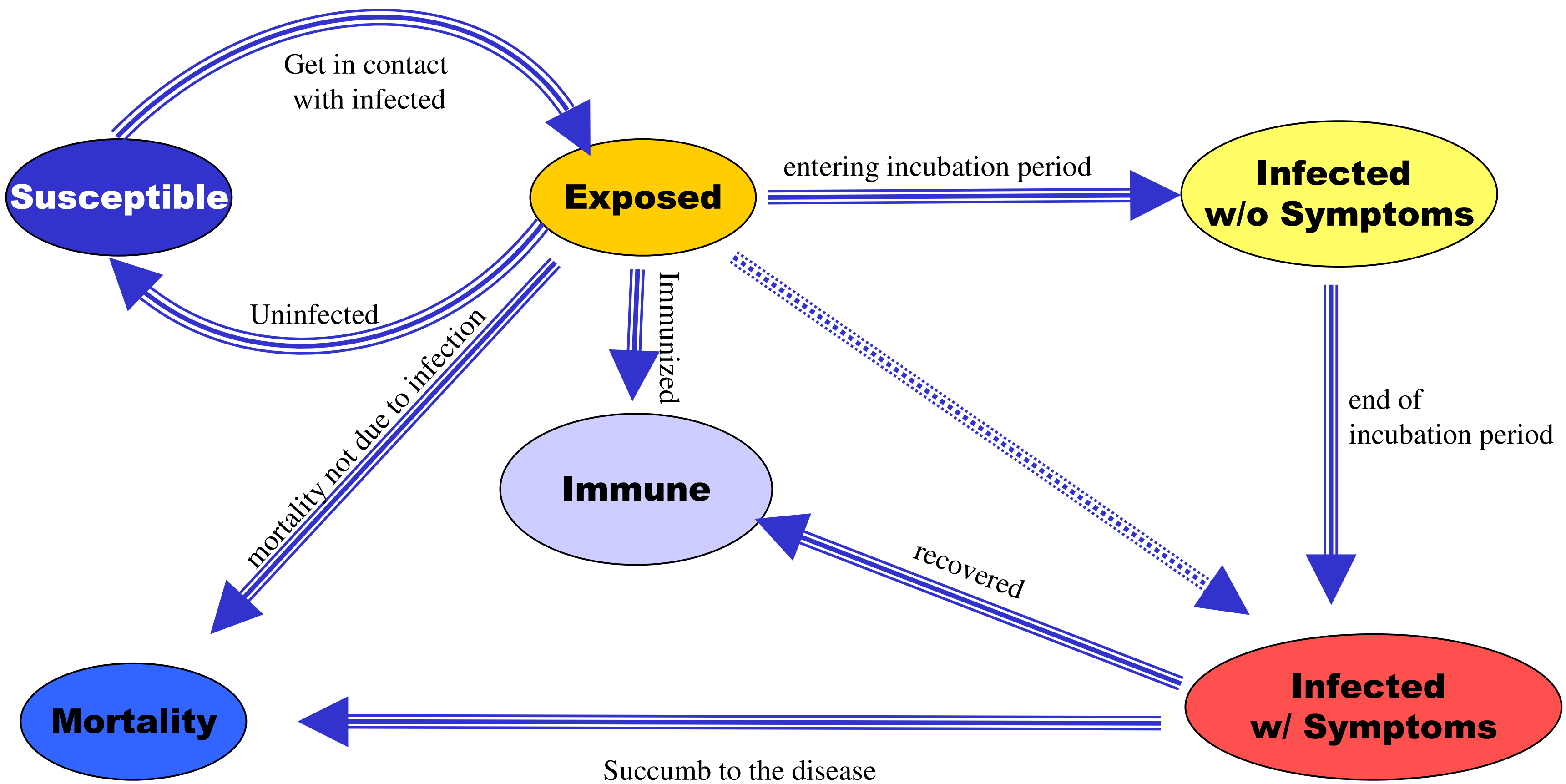
Partners

- Institute for Defense Analyses
- Office of VP IT, Purdue University
- Research and Academic Computing, Indiana University
- Simulex, Inc

Parallel Worlds



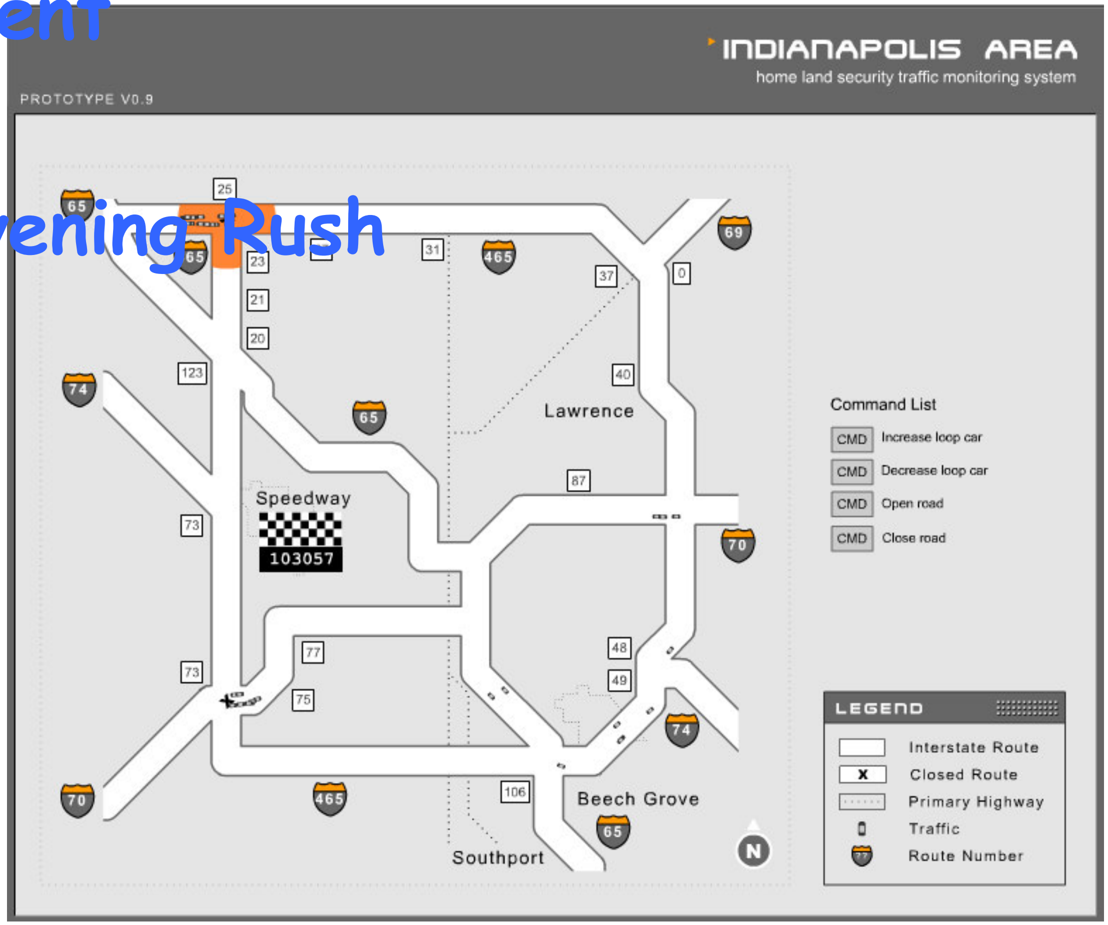
Reproduction Model



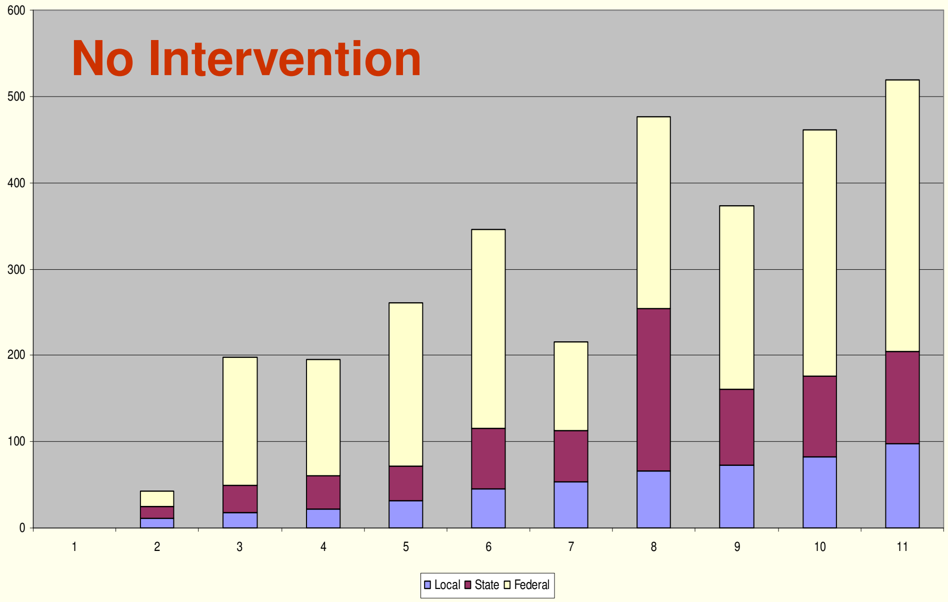
Interventions:
Screen, Isolate (camp or shelter), Treat, Vaccinate

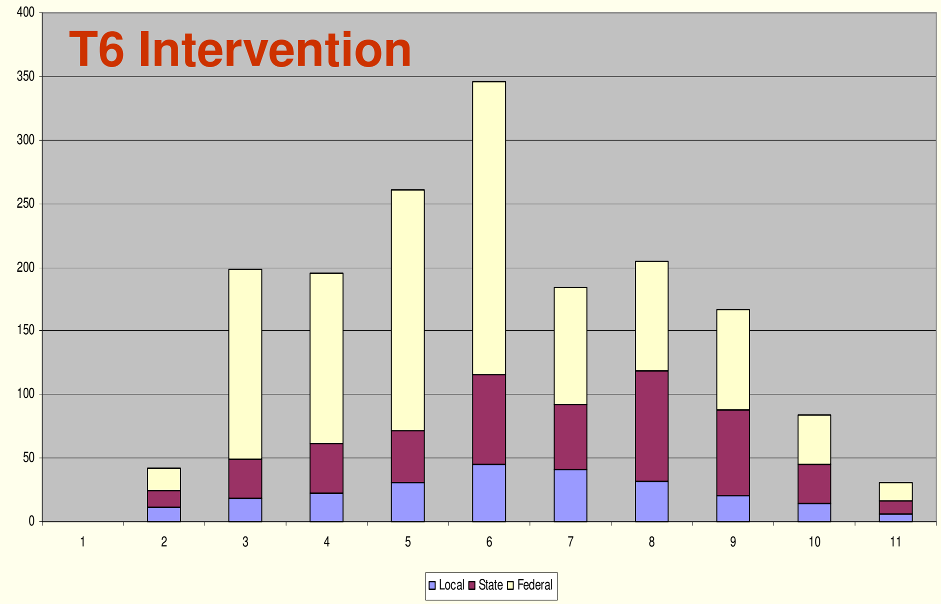
Mobility Models

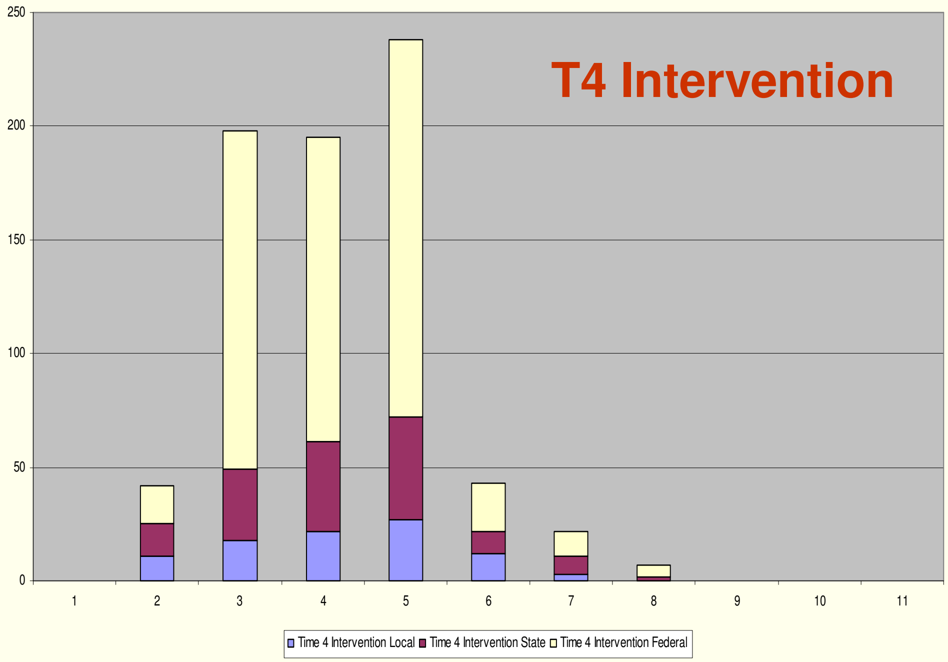
- Regular Movement
- Event Traffic
- Morning and Evening Rush
- Evacuation
- Panic Fleeing

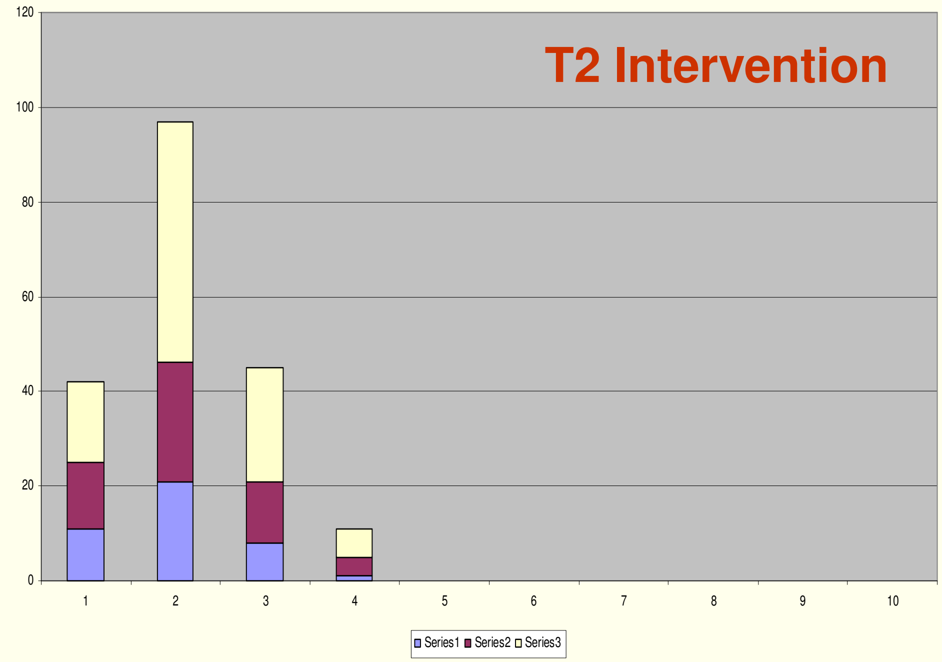


New Infections









Towards a National Grid for HLS