Advanced Scientific Computing for Homeland Security

Steven Ashby

DHS ASC Thrust Area Leader

LLNL Deputy Associate Director for Computation

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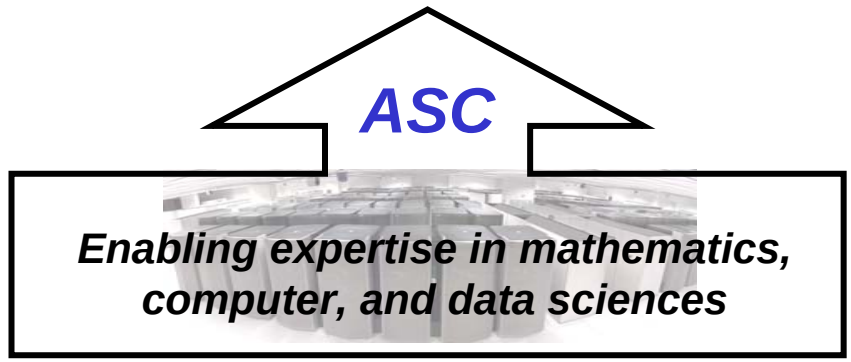
ASC provides computing expertise and capabilities for homeland security

Vision: enable scalable, integrated simulation and information analyses for science-based threat characterization and response

Mission: develop innovative computational technologies for deployment in next-generation homeland security applications

Charter: create enduring capabilities in

- **math, computer science, and scientific computing expertise**
- **modeling and simulation**
- **knowledge discovery**
- **independent evaluations**
- **computational resources**



ASC is engaging customers and reaching out to others to define R&D agenda

- DHS legislation transferred DOE Office of Science *Advanced Scientific Computing Research* activities at LLNL to S&T Directorate

- Defined DHS needs
  - customer and stakeholder interviews
  - Requirements workshop (October 2003)
  - Incident Management workshop (May 2004)
  - Data sciences workshop (September 2004)

- Reaching out to others
  - complementary capabilities at ORNL, SNL, LANL
  - engaging academia and industry

LAWRENCE LIVERMORE NATIONAL LABORATORY

UT-BATTELLE
OAK RIDGE NATIONAL LABORATORY

Sandia National Laboratories

Los Alamos NATIONAL LABORATORY

We organized a workshop to identify relevant computing and math R&D topics

- **Brought together DHS personnel and computing community**
  - **DHS staff from S&T and operational directorates**
  - **leading computer scientists and mathematicians**
  - **academia, national labs, government, industry**
- **Identified where computer science and math R&D could contribute to DHS mission needs**
  - **simulation and modeling**
  - **info mgmt & knowledge discovery**

October 8-10, 2003
Hilton Crystal City

Organized by LLNL and the Krell Institute

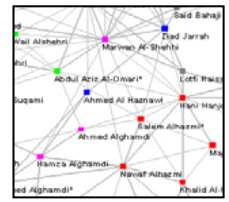
About 80 participants

Preparing report and follow-on workshops

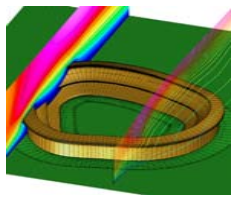
Workshop participants identified numerous ways in which Advanced Scientific Computing can support DHS

Workshops and S&T strategic planning identified four ASC strategic thrust areas

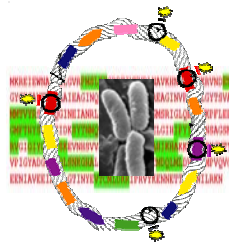
- **Scalable information management and knowledge discovery** for threat identification and risk assessment (enhance ADVISE for IAIP, NBACC, BTS)



- **Integrated simulation analysis capabilities** for threat assessment, training, scenario planning, and incident response (for EPR, IAIP, NBACC)



- **Scalable discrete mathematics** and uncertainty quantification algorithms to enable large-scale multi-simulation and information analyses with confidence measures

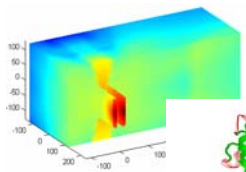


- **High-performance computing resources** for R&D in support of S&T activities and surge capability for DHS operational assets

Enhancing homeland security through simulation and information analyses

- Scenario planning
- Incident response
- Vulnerability assessments
- Source attribution

Simulation for improved emergency response and planning



Enabling expertise in mathematics, computer, and data sciences

Better bio- and radiation detectors for border and transportation security

Scalable information analysis and large-scale data integration

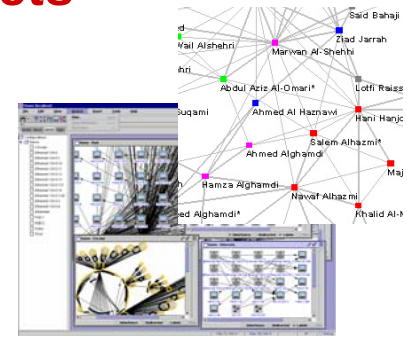
ASC develops new data science capabilities for DHS operational assets

ASC supports DHS customers indirectly by delivering new capabilities to operational assets

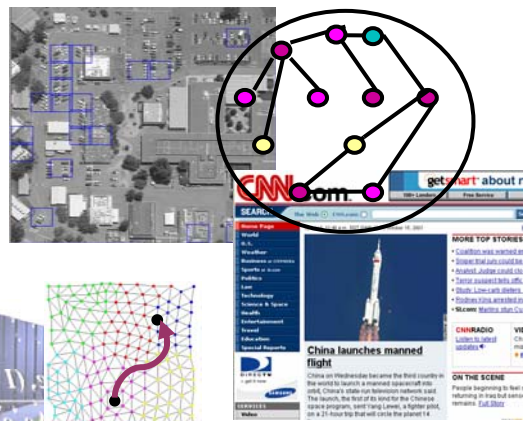
Information Analysis Infrastructure Protection

BKC

ADVISE provides IA and IC analysts with actionable information



These capabilities are integrated into ADVISE



Advanced Scientific Computing Program

ASC researchers develop new knowledge discovery capabilities

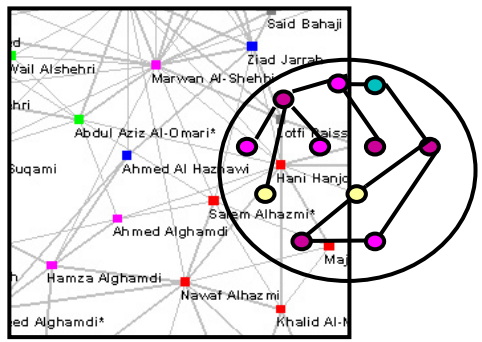
ASC "next generation" capabilities anticipate analysts' needs

ASC is developing scalable information integration and analysis capabilities

Develop ontologies and XML to enable automated access to dynamic, heterogeneous, distributed data sources

Distributed data sources

Integrated, high-level views of data



Incident Analysts

DHS Researchers

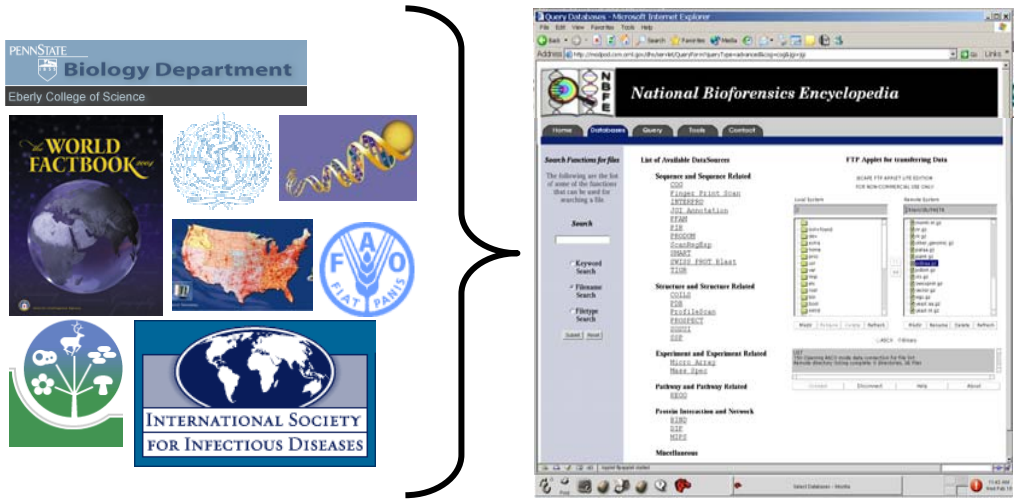
Law Enforcement

***Scalable** classification, clustering, and semantic graph algorithms for **actionable** information analysis*

Provide these capabilities to a variety of users with differing needs

ASC large-scale data integration and querying capabilities enable new BKC

Focusing initial efforts on biology for BKC's Biodefense Encyclopedia



Good example of ASC early research being leveraged into an operational asset

Databases
- Description & schema
- Search across database
- Browse & download

Query
- Query language
- Within & across database
- Keyword search

Tools
- Link web portals
- Tool repository

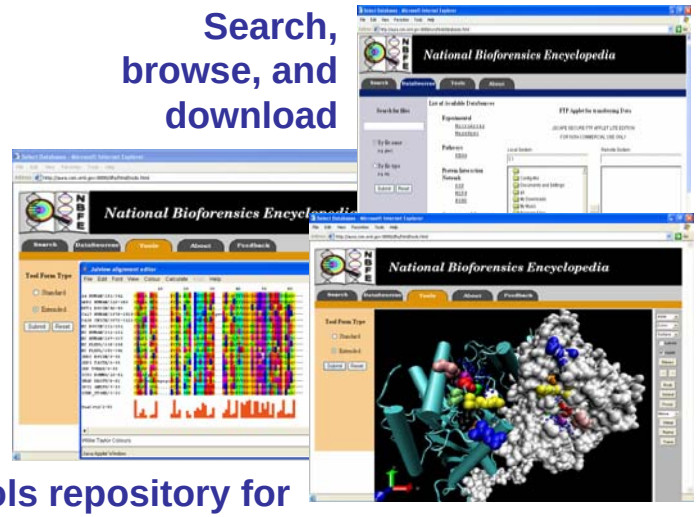
Annotated domain areas
- Biological Agent
- Sequence
- Structures
- Experimental
- Pathways
- Protein interactions
- Miscellaneous

ASC Biodefense Encyclopedia prototype queries multiple data sources

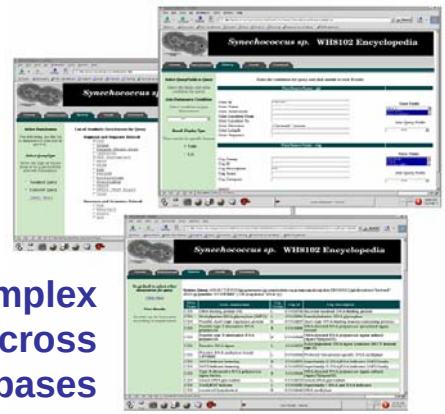
ASC-funded prototype is being modified for use by the BKC

- **Working prototype with 15 integrated genomics and proteomics databases**
- **Preliminary data exchange formats selected**
- **Advanced query language for browsing multiple data sources**
- **Concept-driven keyword extraction from free text data sources (CIA World Factbook, OIE disease cards, FAO, etc.)**

Search, browse, and download

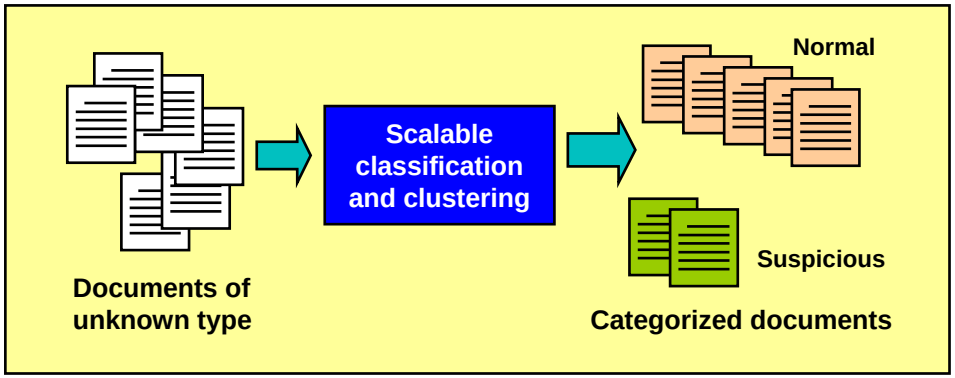


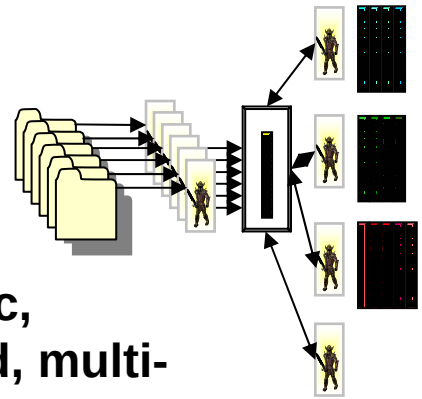
Tools repository for advanced visual analysis



Build complex queries across multiple databases

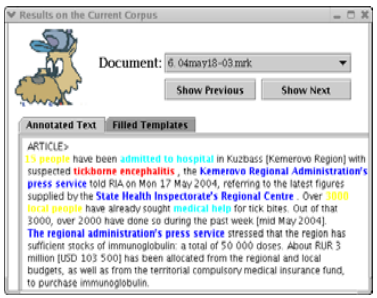
ASC is exploring several approaches to text analysis





2) Dynamic, distributed, multi-agent approach for fast and scalable text analysis

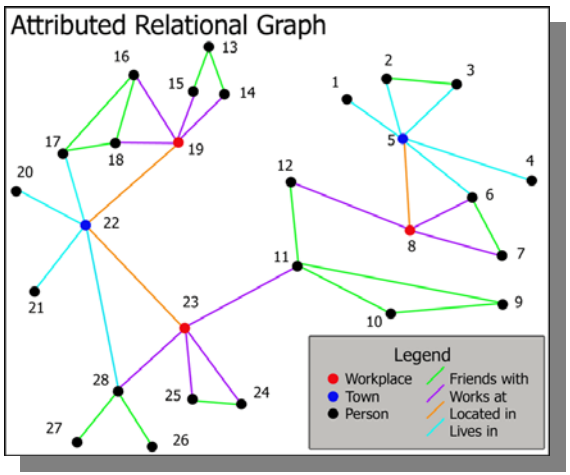
1) Transform free-text documents into semantic data structure for use in ADVISE *(e.g., via Amilcare software)*



3) Investigating utility of IBM's WebFountain software

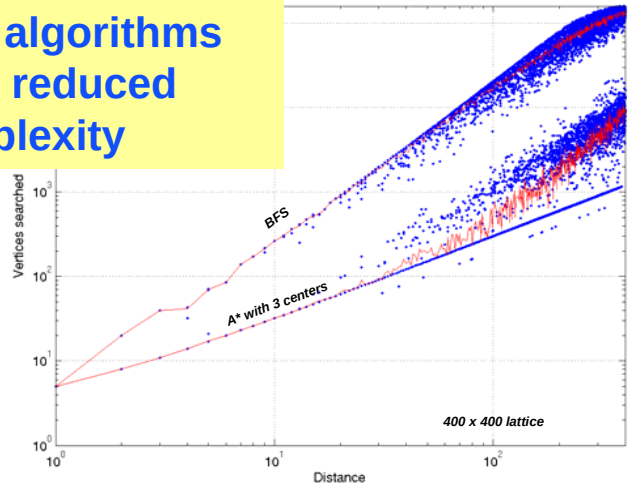
ASC is developing parallel algorithms for scalable information analysis

Semantic graphs are used to represent relationships

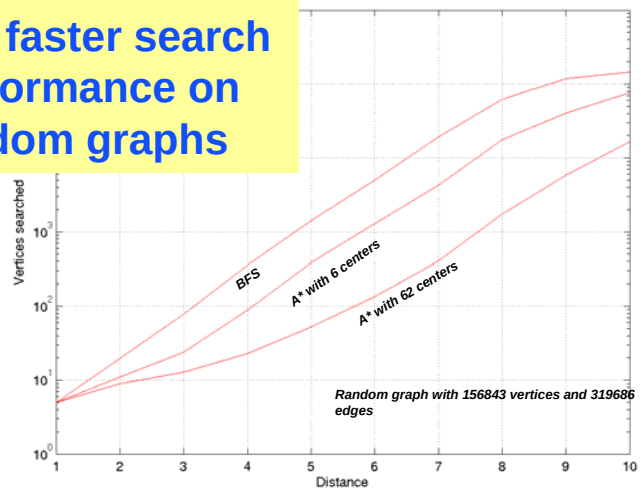


- Huge numbers of edges, vertices
- Ontology-based heuristics for searching semantic graphs
- Scalable parallel implementations

ASC algorithms have reduced complexity

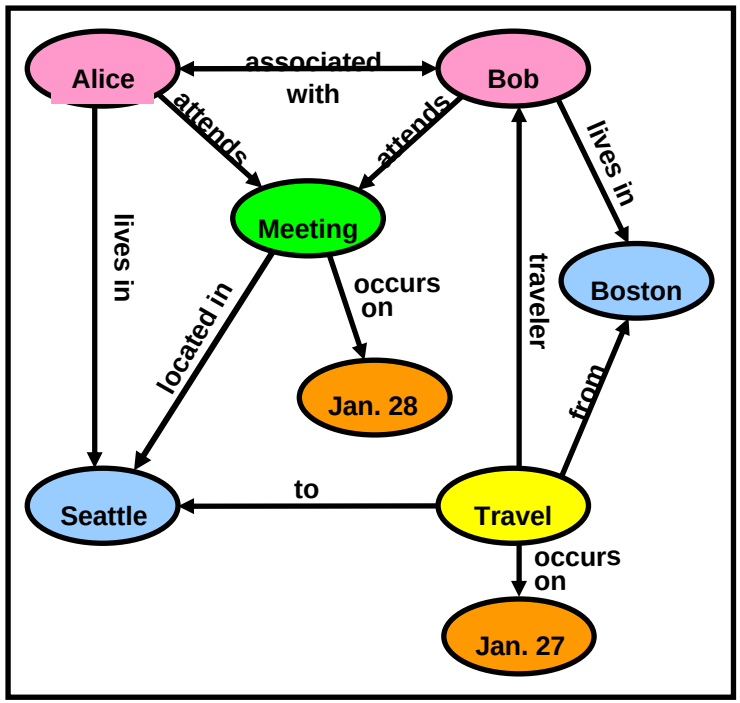


10X faster search performance on random graphs

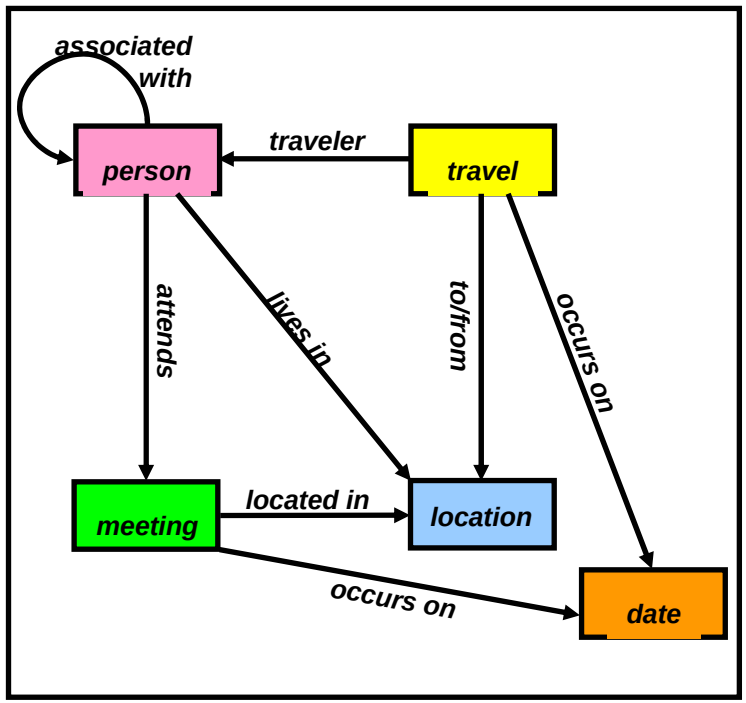


Semantic graphs are used to represent relationships in social networks

Semantic Graph



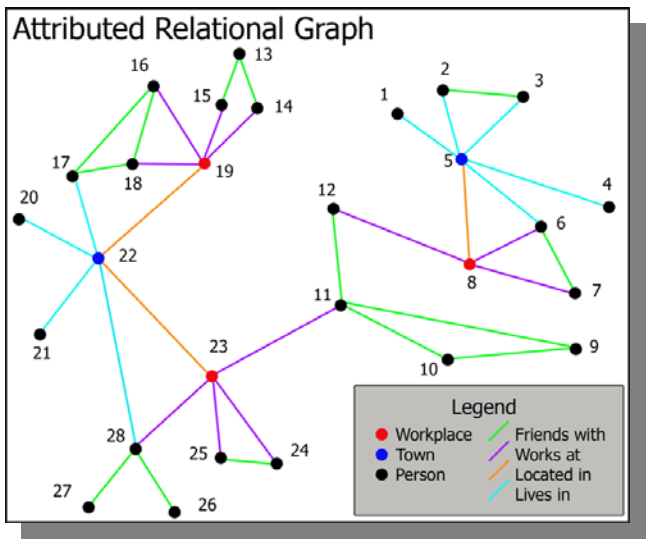
Ontology



Vertices and edges have attributes and types that represent entities and relationships

ASC is developing parallel graph algorithms for scalable info analysis

Semantic graphs are used to represent relationships and to facilitate information analysis

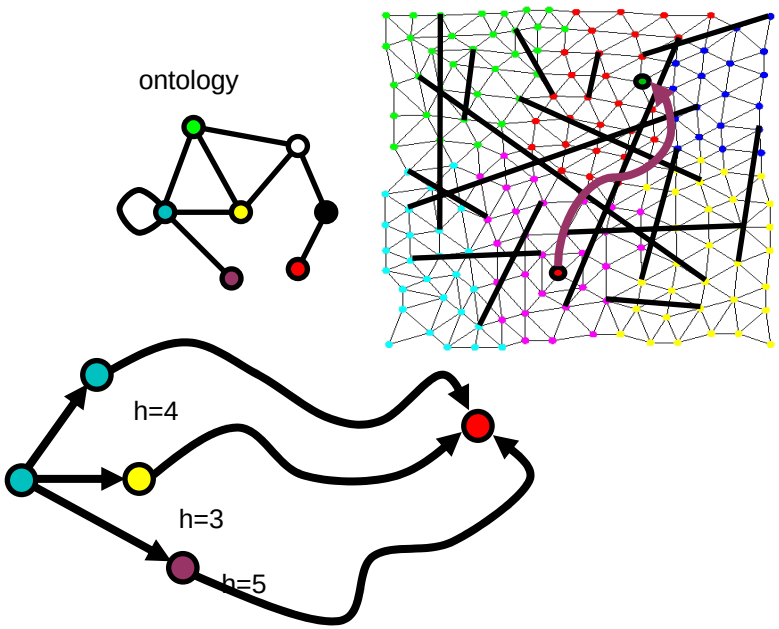


- Parallel computers must be used to store and search large graphs
- Graphs must be partitioned onto separate memories and graph searches must have low cost
- Standard partitioning techniques ineffective for semantic graphs
- We are developing effective partitioners and scalable parallel search algorithms

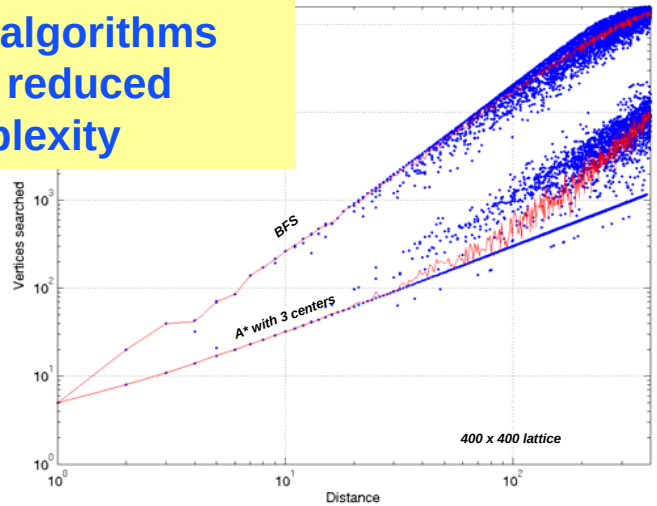
Graphs of interest have huge numbers of edges and vertices

ASC parallel algorithms enable search of massive graphs

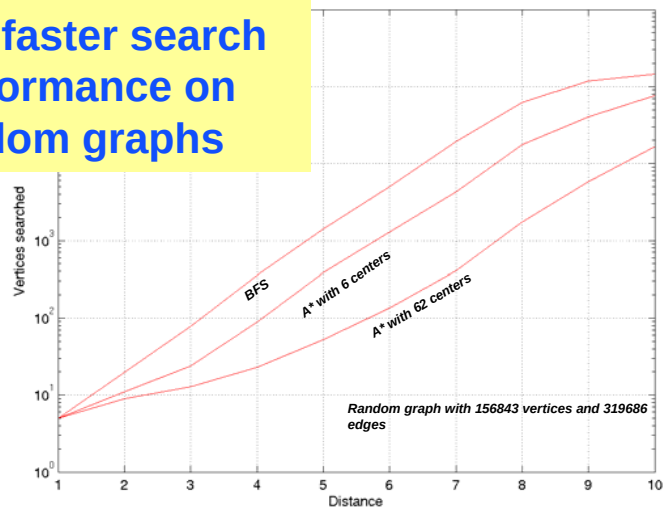
- **Ontology-based heuristics for searching semantic graphs**
- **Scalable parallel implementations**



ASC algorithms have reduced complexity



10X faster search performance on random graphs



Advanced video analysis capabilities could benefit IAIP, EPR, and BTS

Solved problem

High resolution
~1 cm/pixel
Small FOV

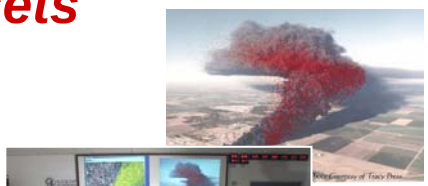
Moderate resolution
~20 cm/pixel
Moderate FOV

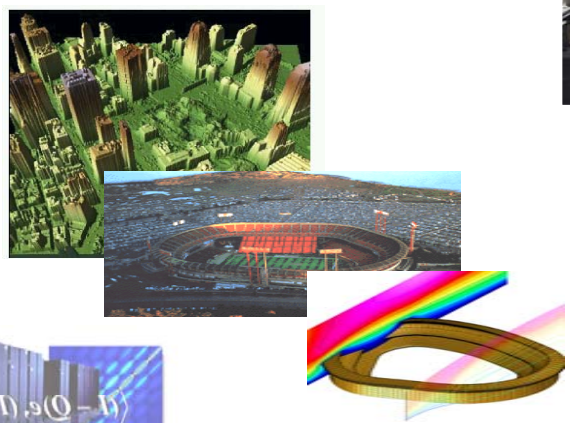
Low resolution
~1 m/pixel
Large FOV

- **Myriad applications (monitoring troop movements, video surveillance, etc.)**
- **Scalable feature extraction and change detection algorithms**
- **Faster, more accurate, and more robust performance**

ASC develops new modeling & simulation capabilities for DHS operational assets

ASC supports DHS customers indirectly by delivering new capabilities to operational assets





IMAAC provides FEMA and first responders with better plume predictions

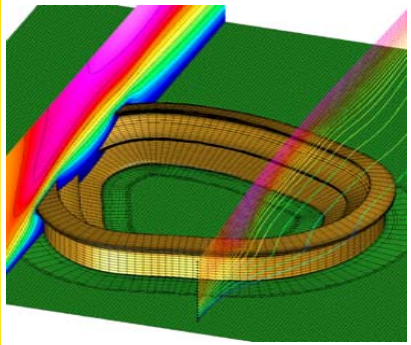
These capabilities are integrated into IMAAC codes

ASC researchers develop new modeling and simulation capabilities

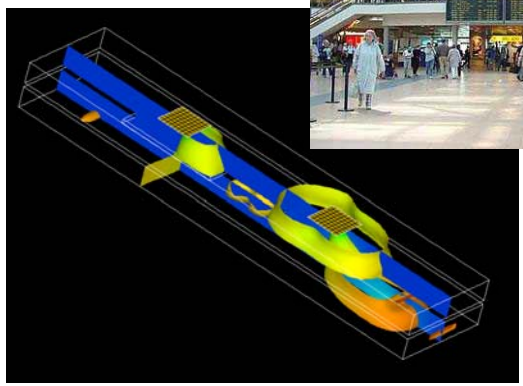
ASC "next generation" capabilities anticipate first responder needs

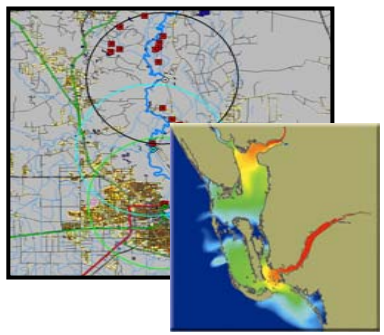
Accurate CFD capabilities for dispersion modeling in air, water, indoor facilities

Advanced meshing and complex geometry capabilities for atmospheric release codes



Modeling of indoor flow and transport of chemical and biological agents

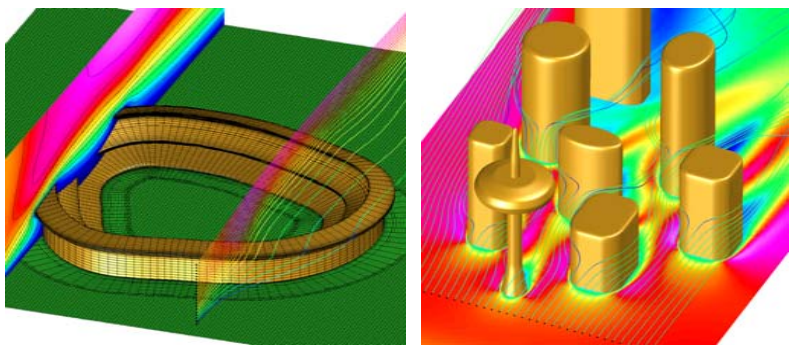




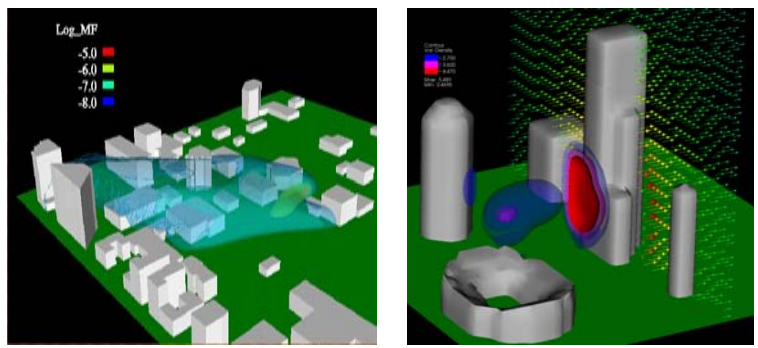
Modeling of surface-water transport of nuclear, chemical, and biological agents

ASC is developing new capabilities for aerosol modeling in urban settings

- High-fidelity, computationally efficient dispersion simulations are useful for scenario planning and incident response
- We are developing advanced meshing and complex geometry capabilities for atmospheric release codes
  - automatic geometry-to-solution capability
  - adaptive mesh refinement for enhanced resolution and multi-scale phenomena



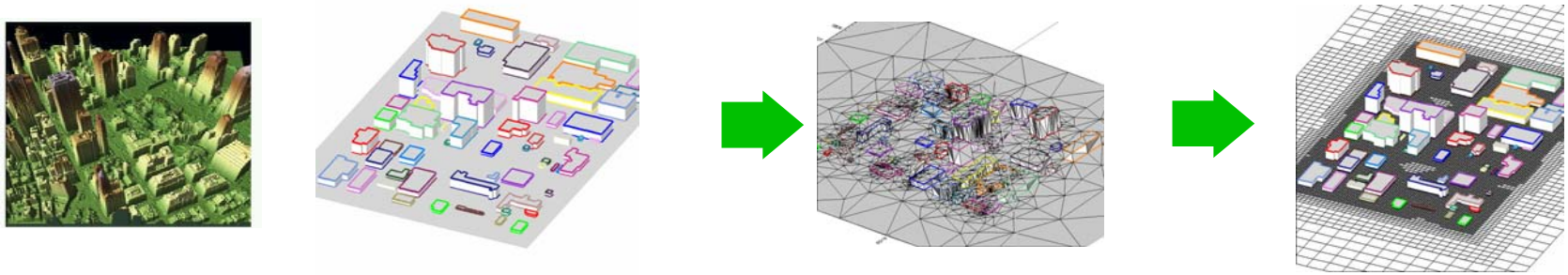
3D flow over stadium and cityscape



3D flow calculations over cityscape

ASC automatic grid generation approach is 5000X faster for incident response

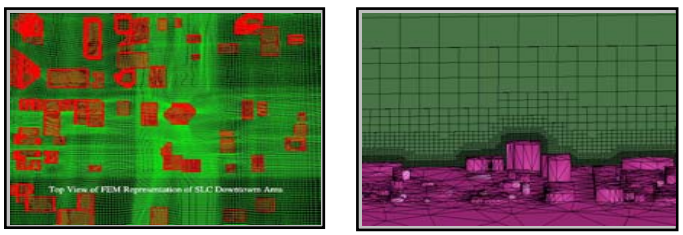
Goal: Building geometry to high-fidelity simulation *automatically*



Early success

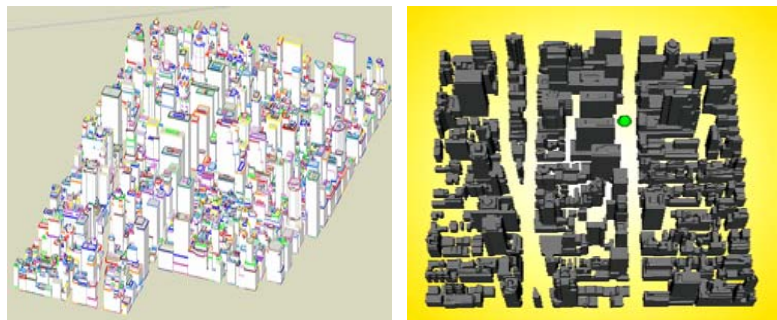
Reduced problem setup time from 1 week to 2 minutes 5000X

Downtown SLC with 60 buildings (for 2002 Olympic Games)

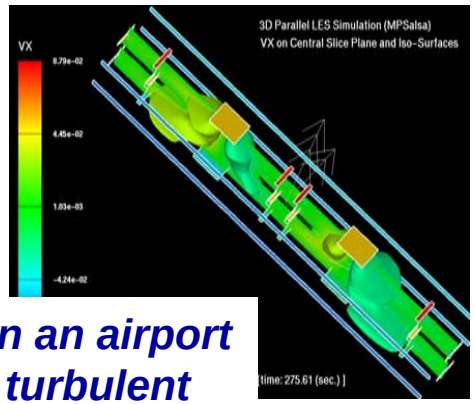


Manhattan study

ASC approach *essential* to modeling of 3600 buildings



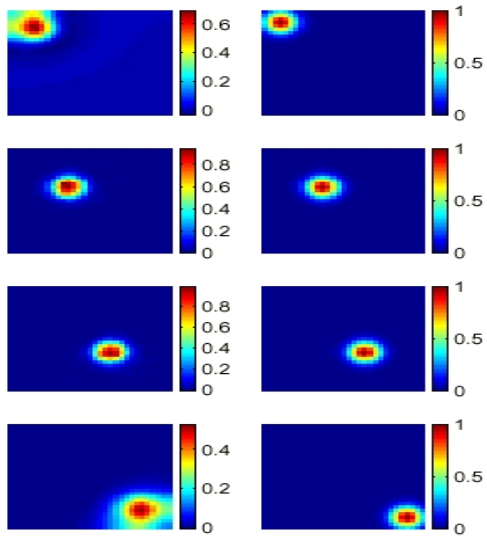
ASC is developing indoor dispersion modeling and source inversion methods



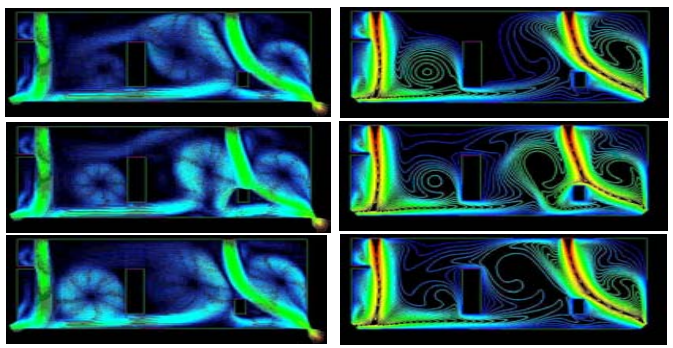
Chemical attack in an airport terminal via 3D turbulent flow simulations

- High-fidelity indoor dispersion simulations
- Source inversion and optimal sensor placement
- Decontamination studies

Inverting for Location of a Moving Chemical Source



Decontamination study: transient infusion of ClO_2, H_20 to neutralize anthrax

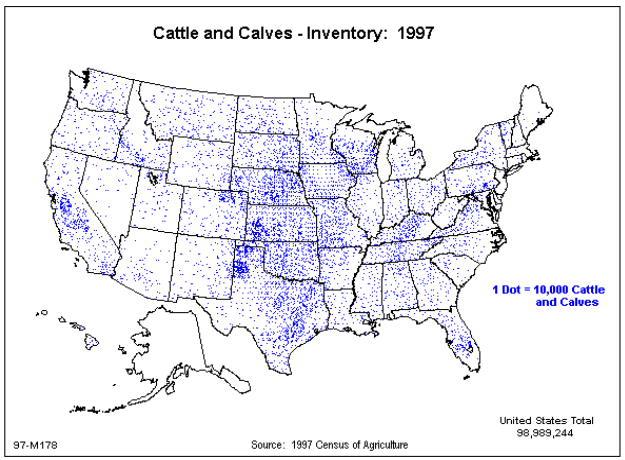


Velocity Vectors ClO_2 Contours

ASC will explore algorithmic and software issues in agent-based modeling

- Agent-based modeling is increasingly important for DHS program areas
  - Motivation & Intent
  - CIP-DSS (CIP)
  - FMD-DSS (Bio)
  - NIMS (EP&R)

Application: Disease spread

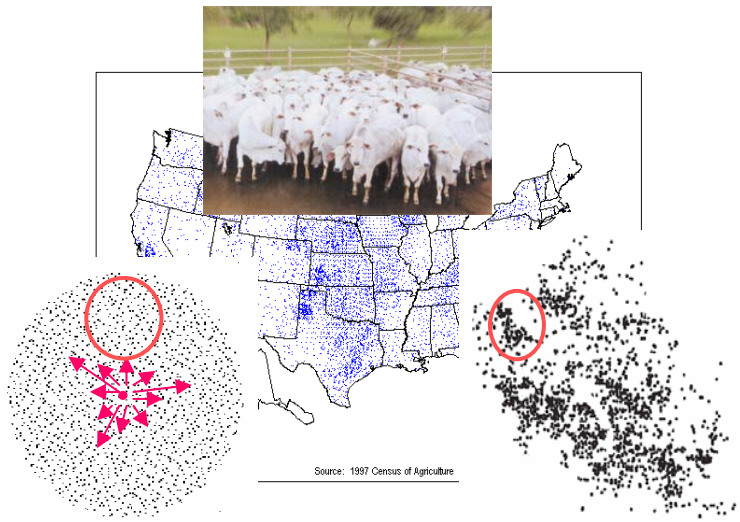


Application: Impact of terrorism on economy

- Partner with customers to identify R&D challenges
- Workshop later this year

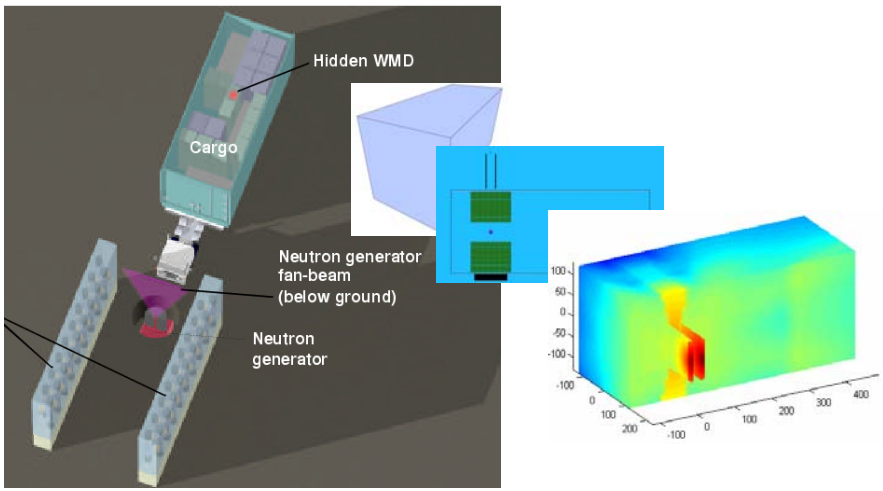
New epidemiological models and discrete simulation of disease spread

- Goal: analyze an epidemic and predict its spread
- Use modeling and simulation
  - Devise control strategy and plan resource distribution
  - Identify initial source(s)
  - Improve infectious disease spread management practices
  - Train personnel
- DHS request: focus initially on FMD
  - Develop appropriate epidemiological model
  - Implement in a scalable simulation framework
  - Collaborate with academia
- Key first step: gap analysis via evaluation of existing efforts
  - Strengths and weaknesses
  - Needed computing R&D
  - Presented results to DHS on July 22, 2004

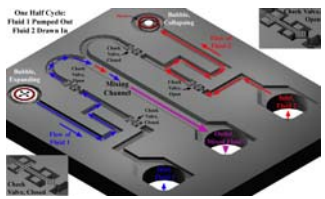


ASC modeling enables design of more effective radiation and bio- detectors

Radiation transport modeling determines best source/detector configuration for cargo container inspection



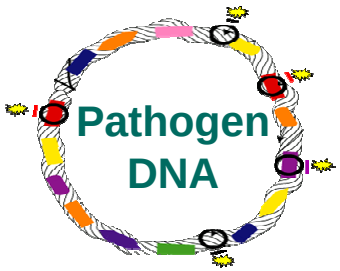
10X faster and more robust pattern recognition algorithms for DNA signatures for BioWatch system



Computational bio-fluidics is used to improve next generation bio-detectors

ASC researchers delivered 10x speedup in DNA signature algorithm

DNA signatures are key to pathogen detection



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aaag.cacttcc..at.ga.ta.gg.actgggtttta.aaacctgtgatgg
c.tc.aagaccct.gaggc.ATCCTCTC**CTTTGCACGCC**
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.TGGGTGAACGCCGTGTGCGG.gacg...aa

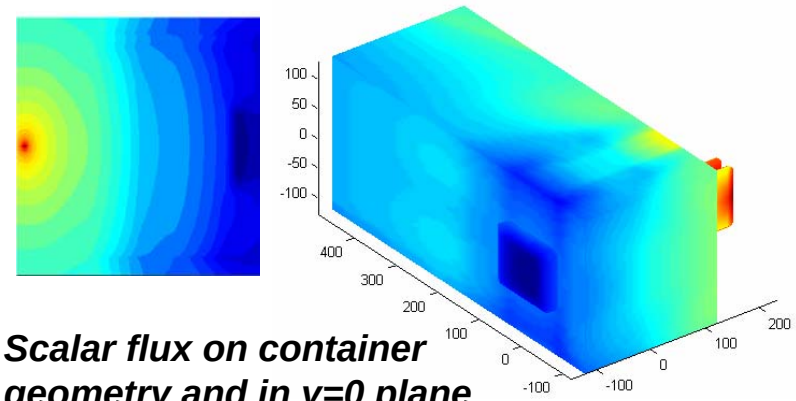
Pathogen DNA sequence

Identify unique DNA signature via sequence alignment algorithms

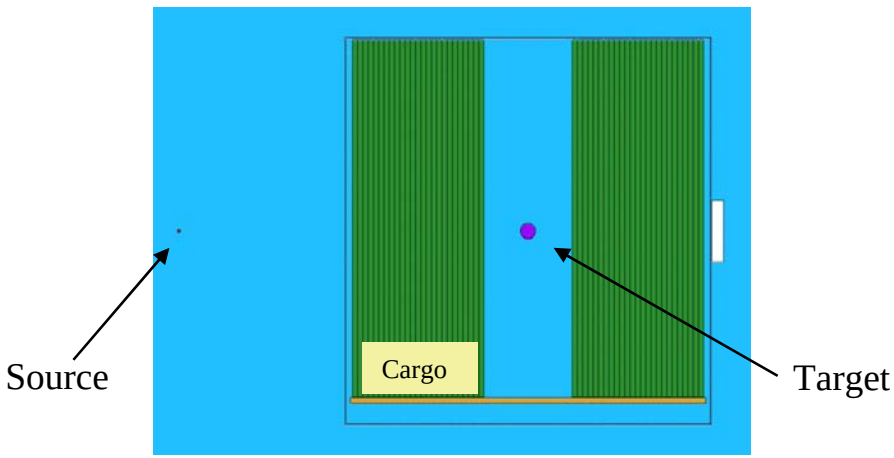
- **ASC developed new sequence alignment algorithms and delivered to biodefense program**
  - **10x faster algorithm greatly speeds development of DNA signatures for pathogen detectors**
  - **New algorithm is the first ever to work on draft sequences (major contribution to the field)**

Deterministic radiation transport enabled design of sensors for cargo inspection

- **Ardra simulations now include delayed neutron data**
- **Initial 3D simulation qualitatively matches Monte Carlo code**
- **Validation studies underway**

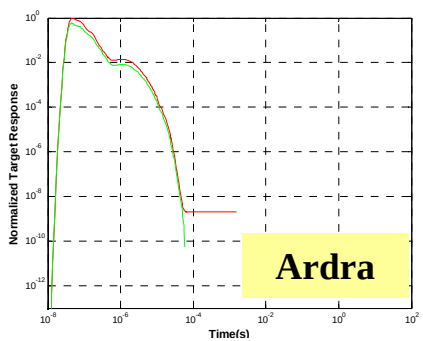


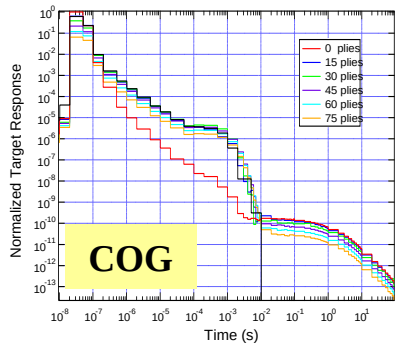
Scalar flux on container geometry and in y=0 plane



Vertical section of cargo container model geometry in y = 0 plane

HEU Target Response Time Evolution With and Without Delayed Neutrons

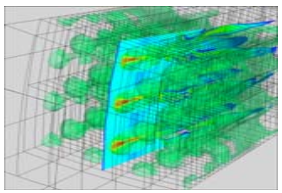




Advanced simulation capabilities could benefit IAIP, EPR, and BTS

Couple shock and structural simulation codes to understand blast effects and natural hazards

Couple with dispersion modeling for consequence analysis



Customer: CIP
(in partnership with CIP-DSS)

Develop new capability to quickly and accurately model the effects of Radiological Dispersion Devices

<u>RDDs present many challenges</u>

- **Dispersion modeling**
- **Decontamination studies**
- **Aerosolization**
- **Particles of varying sizes**
- **Chemical interactions**

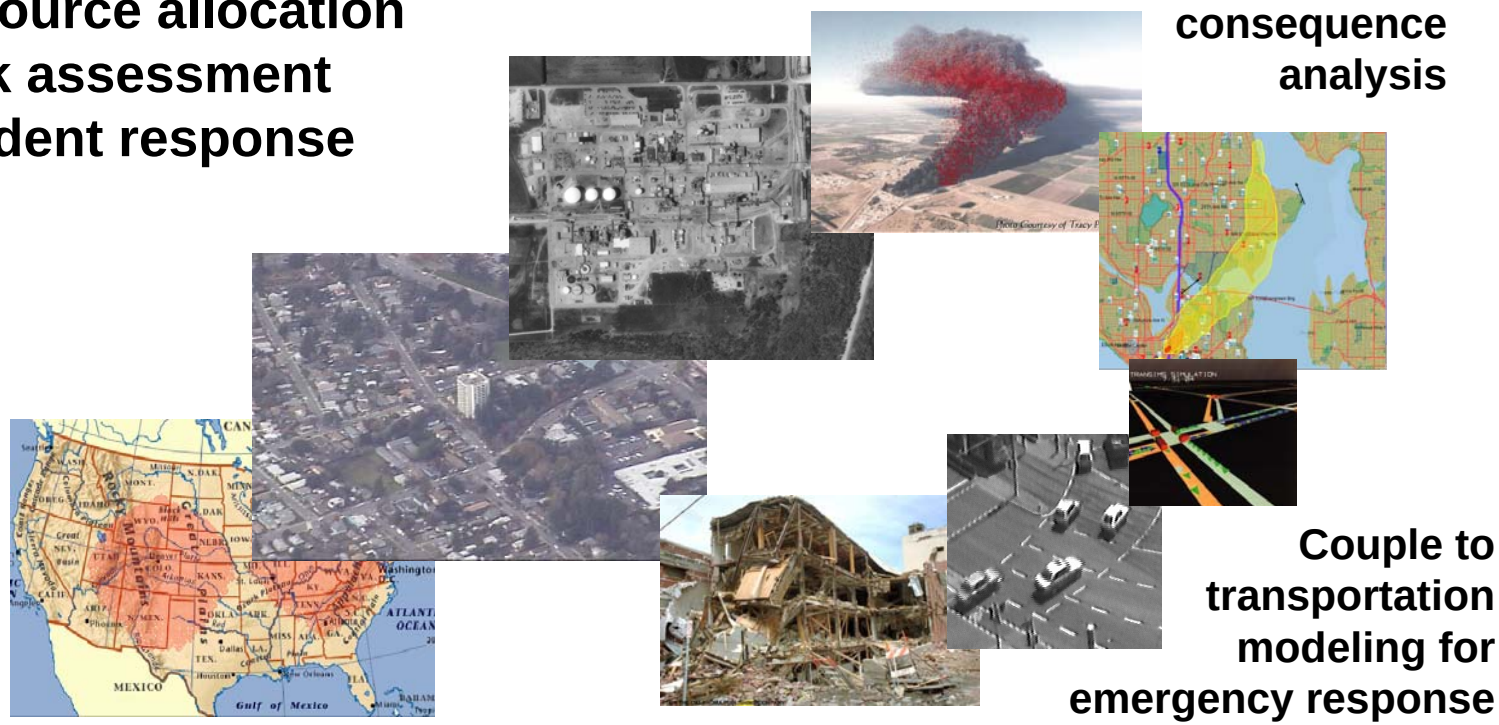
Customers: EPR, BTS

ASC's vision is to integrate these capabilities into decision support tools

Teaming with others to define a National Incident Management decision support framework

- Local, regional, national levels
- Training and scenario planning
- Resource allocation
- Risk assessment
- Incident response

Couple with dispersion modeling for consequence analysis



Couple to transportation modeling for emergency response

We are leveraging LLNL's world-class computing resources to benefit DHS

- ASC invested FY03 funds in LLNL's institutional computing program

- Provided access to LLNL high-performance computing resources
  - 23-teraflop Thunder Linux Cluster and smaller capacity machines
  - available to all DHS personnel
  - classified resources available

- Livermore Computing (LC) offers outstanding 24x7 customer support
  - hotline call center
  - education and training

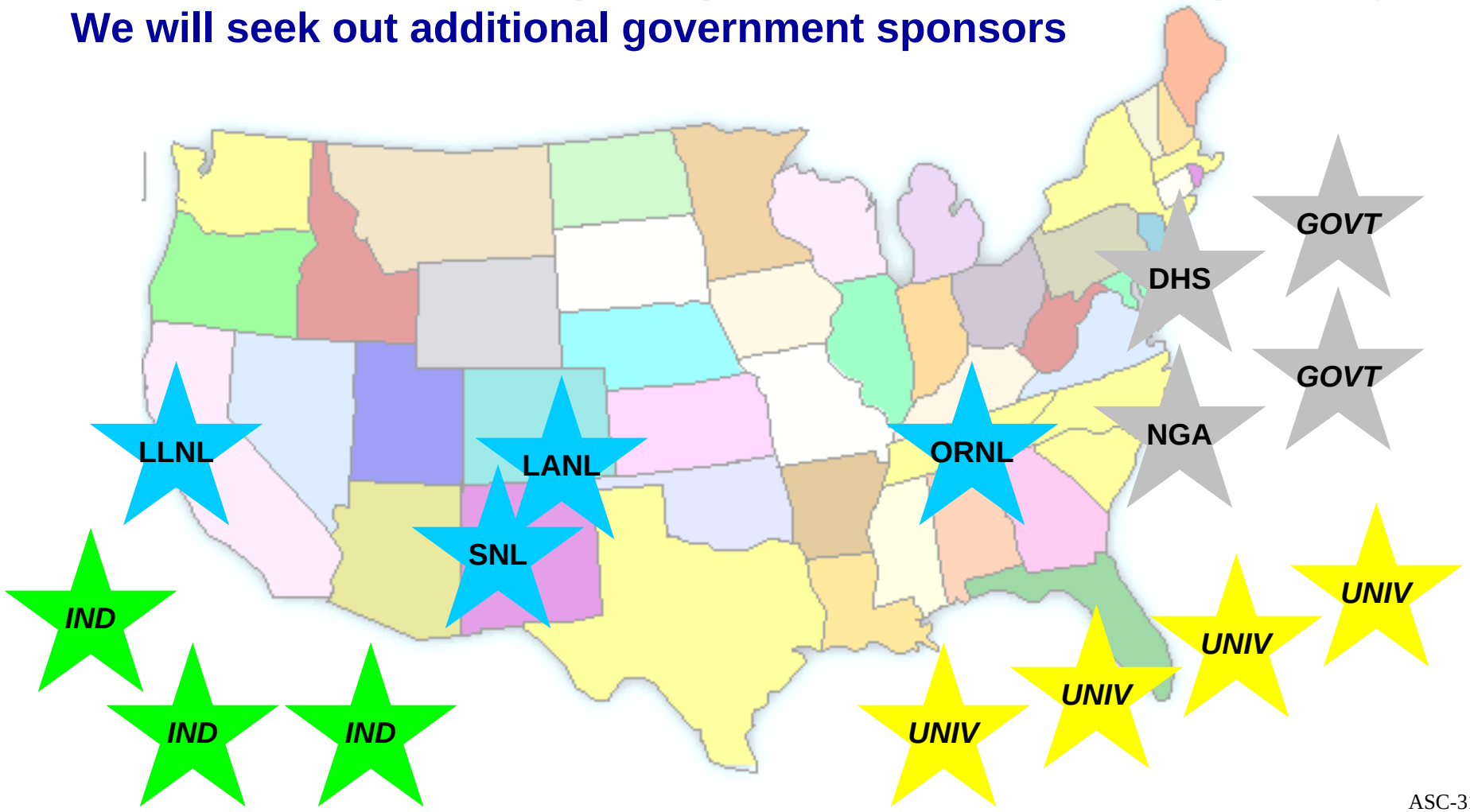
DHS is forming a national Institute for Discrete Sciences

- IDS will conduct R&D in areas important to DHS
  - Large-scale information management
  - Scalable knowledge discovery
  - Discrete mathematics and simulation

- Creating a national research partnership to fill a gap in the federal research portfolio
  - National laboratories (applied R&D)
  - Academia (fundamental research)
  - Industry (applied R&D and tech transfer)
  - Other agencies (broader impact and interactions)

IDS will bring together lab, academic, industry, government participants

Academic and industrial participants will be chosen competitively
We will seek out additional government sponsors



IDS will be a true partnership, not a collection of researchers

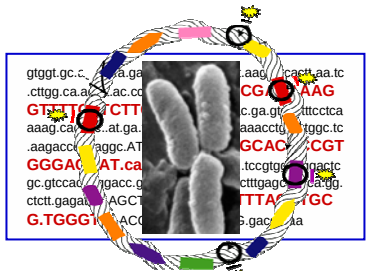
- Academic partners
  - Basic research
  - Students and postdocs
  - Education & training
  - Linkage model being developed
- Lab partners
  - Applied research
  - Advanced development and deployment
- Industrial partners
  - Directed R&D
  - Commercialization as appropriate

- Integrated teams
  - Multi-institution
  - Collaborative research and joint publications
  - Residential visits (at labs) by students and faculty
- Real deliverables
  - Longer term R&D focused on identified needs
  - Clear “insertion paths” into operational assets

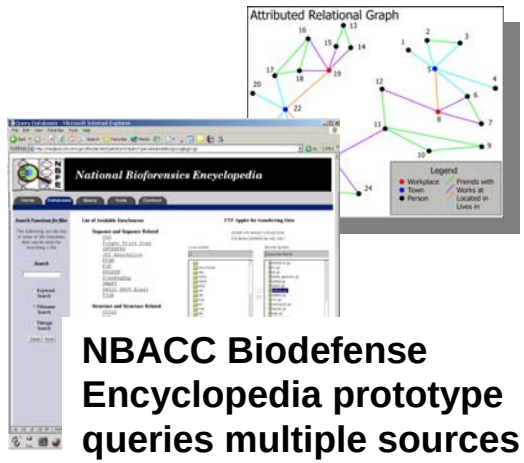
Key objective: ensure strong coupling of all elements and participants

Summary: ASC is developing new capabilities for homeland security

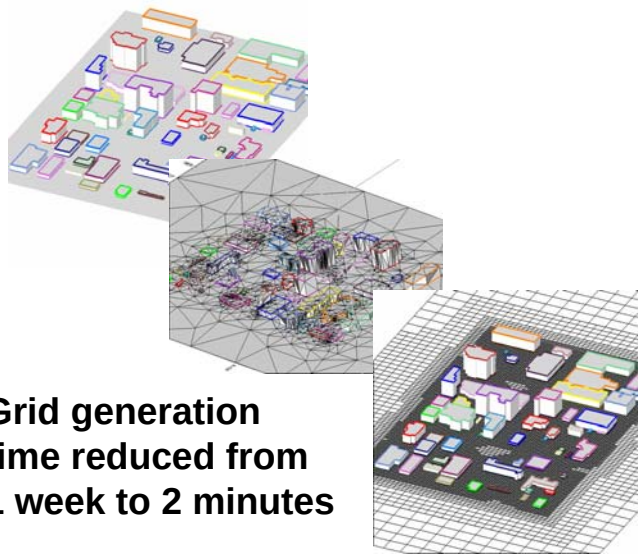
ASC Requirements Workshop defines program



10X faster and more robust DNA signature algorithms delivered to CBNP

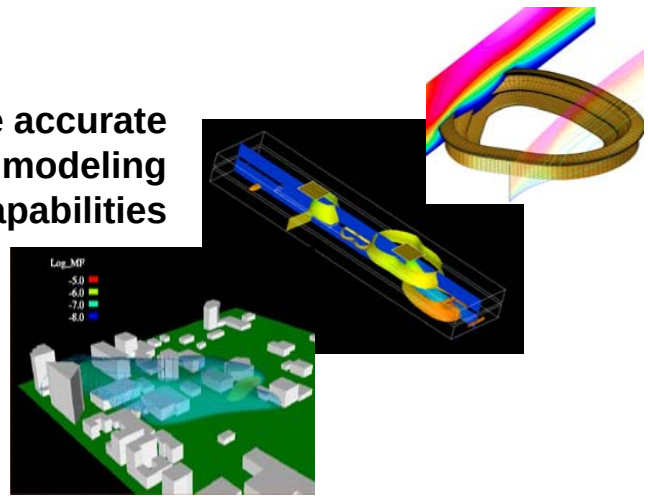


NBACC Biodefense Encyclopedia prototype queries multiple sources



Grid generation time reduced from 1 week to 2 minutes

More accurate dispersion modeling capabilities



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