Threat Agent Science Capability Area

Computational Chemistry Thrust Area

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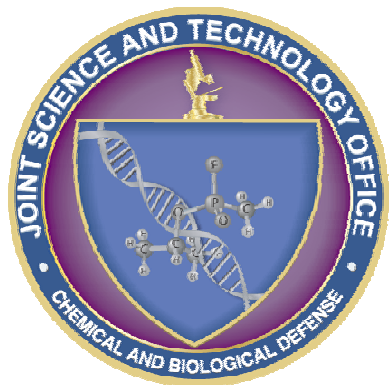

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Overview

- Organizational Overview
- New Computational Chemistry Thrust Area within the Threat Agent Science Capability Area Focus Areas
- Potential applications
- Current efforts
- Planned thrusts

JSTO Organization

Physical Science & Technology Division

- Detection
- Protection
- Decontamination
- Mod., Sim., & Battlespace Awareness
- Threat Agent Sciences

Program Integration Division

Medical Science & Technology Division

- Pretreatments
- Therapeutics
- Diagnostics
- Emerging Threats

Applied Technology Division

CAPOs empowered to make program decisions

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TAS Capability Area

Threat Agent Science
Dr. Dave Stockwell, CAPO
JSTO (DTRA/CBT)

- **Agent Fate**
  Dr. Jim Savage
  ECBC
- **Low Level Tox.**
  Dr. Steve Channel
  AFRL @ ECBC
- **Agent Characterization**
  Simulant Development
  Dr. Jon Kaufman
  NAVAIR
- **Computational Chemistry**
  Dr. Paul Murdock
  AFRL
- **Science Info Support**
  Ms. Deb Schnelle
  DTRA/CBT

AFRL Organization

HQ AFMC
Material Developer

- Headquarters
- Field Operating Agencies
- Air Logistics Centers
- Product Centers
- Test Centers
- Air Force Research Laboratory
- Specialized Product Centers

Human Effectiveness Directorate
AFRL/HE

Biosciences and Protection Division
AFRL/HEP

CB DEFENSE TEAM
AFRL/HEPC CBD

AFRL CHEM & BIO DEFENSE (CBD) TEAM

HUMAN EFFECTIVENESS DIRECTORATE
BIOSCIENCES AND PROTECTION DIVISION
COUNTERPROLIFERATION BRANCH

AFRL/HEPC

- **JSTO EXECUTION**
- **JOINT COMMUNITY MEMBERSHIP**
- **AF's CB DEFENSE "ANSWER SHOP"**

Computational Chemistry Thrust Area

Objective

Develop and apply quantitative chemistry techniques and tools to provide accurate technical threat agent understanding and prediction

- Agent Fate on complex surfaces
  - i.e. concrete, asphalt, grass, sand, other operational surfaces
- Address emerging and new threat agents
- Agent/Simulant correlation and simulant design
- Application to agent toxicology and hazard
- Decrease dependence on empirical testing and infrastructure

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Potential Applications of Computational Chemistry

- Assist in the Development of Accurate Models of Chemical Hazard Persistence and Risk Duration
- Chemical Agent Fate
  - Live Agent Tests are Expensive
  - Facilities Scarce
- Simulant Correlation
  - Design?
- Provide Insight into Chemical Agent Interaction with Surface Materials
  - What happens to the agent?
  - What "liberates" the agent from the substrate?
- Individual and Collective Protection
- Decontamination Issues
- Operational Considerations
- Toxicological Effects

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Computational Chemistry Thrust Area

- Two Focus Areas
  - Quantitative Structure Activity Relationships (QSAR)
  - Quantitative Chemical Theory (QCT)
  - Possible additional areas per proposal inputs
- QSAR
  - CBRTA Independent Assessment and Evaluation of QSAR in Predictive Modeling underway (Cipher Systems, SRC)
  - Results delivered
- QCT
  - FY06 New Start
  - Performers
    - Naval Research Laboratory (Dr. Bermudez)
    - AFRL (Mr. Kilpatrick, Dr. Evans)

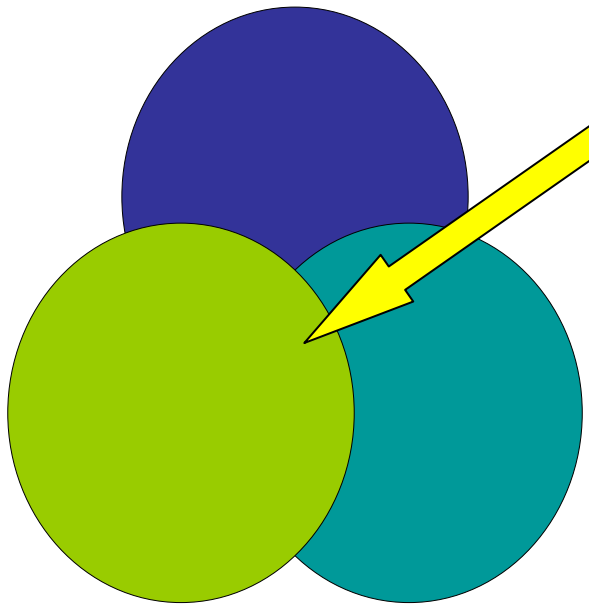
Quantitative Structure Activity Relationships (QSAR)

- Problem
  - Efforts to “improve” simulants will result in more toxic simulants (Similar Property Principle)
  - Efforts to “improve” simulants still won’t accomplish the goal of the Thrust Area
- Emphasis should be on understanding *correlation* between simulant activity and agent activity, and using this understanding to make predictive statements about agent activity

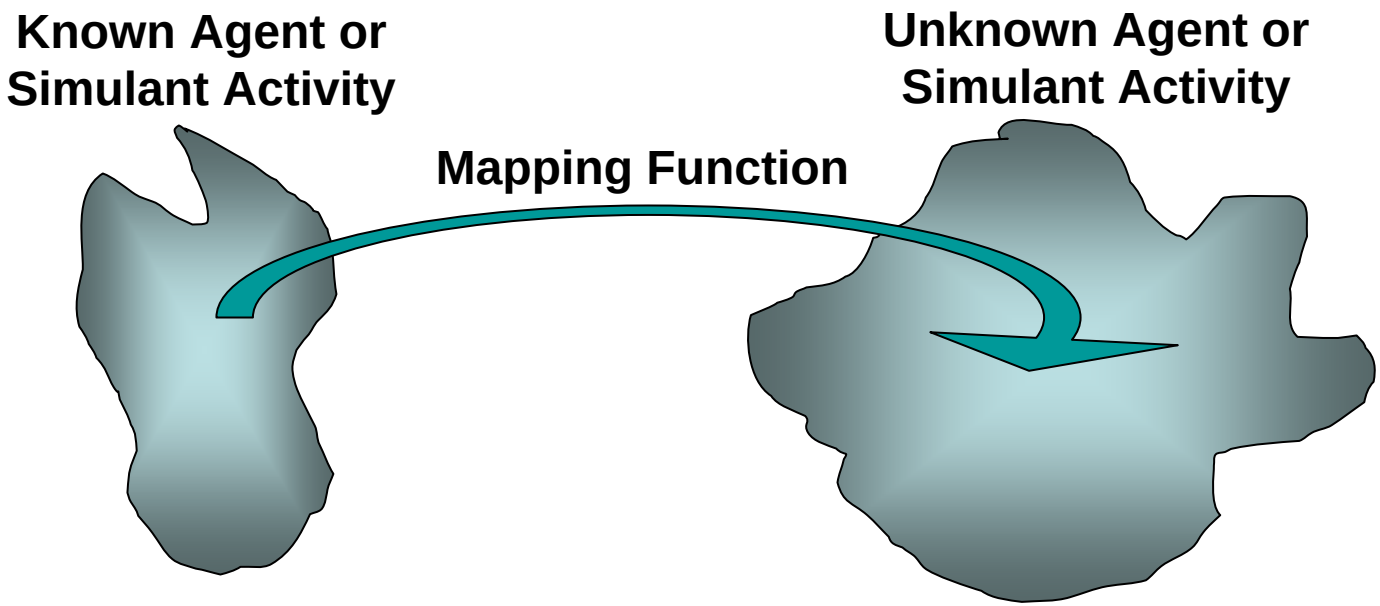
QSAR
Understanding Agent and Simulant Activity

- Use a combination of experimental and computational methods, in connection to QSAR
- Determine the correlation between agent/simulant structure and SPECIFIC activity
- Create mapping functions to map known simulant activity into set of unknown agent activities

QSAR
Understanding Agent and Simulant Activity



QSAR
Predicting Agent Activity



Quantum Chemical Theory (QCT)

- Problem
  - Shortcomings of experimental approach to agent/surface interaction investigations
    - Too many permutations
    - Risk and cost associated with agent experimentation
    - Rate of emerging threats faster than traditional empirical approach can accommodate
  - Extensive reliance on simulants to represent CWAs
- QCT is a readily available technology
  - First principles approach to understanding agent/surface interaction effects
  - Does not replace experimental efforts
  - Only possible given recent HPC improvements
    - SGI Origin 3900 (128 MIPS R12000 CPUs, 256 Gb memory)
    - Year 1 effort is ~ 50,000 CPU hours

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Quantum Chemical Theory (QCT)

- QCT tools have been extensively developed and thoroughly tested by academia
  - No new software tools needed
  - Application to CWAs is direct extension of existing work
- New start effort
  - Joint AFRL and NRL project
  - Incremental approach to validate application of QCT modeling to agent fate and agent/simulant correlation
    - FY06: Validate quantitative reliability of QCT against simulant data
    - FY07: Evaluate extent of currently used simulants to reproduce properties of CWAs; begin calculations on agent surface interactions with solid oxide surfaces
    - FY08: Extend modeling of CWAs absorbed onto solid oxides to complex surfaces
  - Broad application to other areas within CB defense

Current Efforts

- Expansion of the Computational Chemistry Thrust Area
- Evaluation of Proposals for FY07 Start
  - Responses to JSTO Service Call
  - Responses to JSTO BAA For Industry

Computational Chemistry Thrust Area

Questions?

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