### Overview of US Army ERDC Environmental Risk Assessment Research

Presented to

USEPA ERAF and TSERAWG
Joint Winter Meeting
January 27, 28 and 29, 2009
Vicksburg, MS



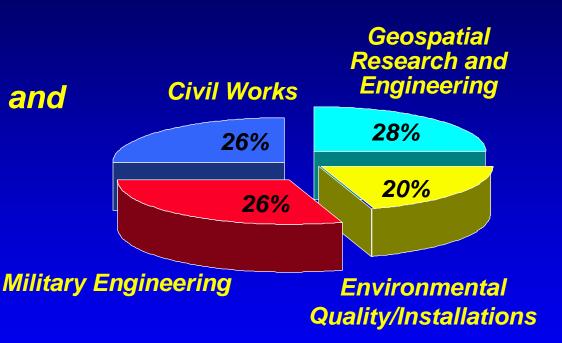
### Engineer Research and Development Center





### ERDC FY08 Program

- > Environmental Quality/Installations
- > Military Engineering
- Geospatial Research and Engineering
- Civil Works Water Resources



FY 08 Total Obligation Authority \$1.3B

- 75% Reimbursable
- 25% Direct



### The future of risk assessment!

- Increased understanding of the toxicological mechanism -- from the molecular scale to population scale.
- Improved understanding of biological availability and how contaminants move through ecosystems.
- Ability to predict bioavalability and toxicity via molecular structure.
- Improved visualization tools, enabling risk managers, stakeholders and the public to better understand risk and facilitate decision making under uncertainty.



### How are we getting there!

- Toxicogenomics
- Biological Network Science
- Computational Chemistry and Biology
- Emerging Contaminants –
   Nanomaterials, PEP, etc.
- Distributed Source Analysis Range Sustainability



### Basic Research

- -Environmental Sensing/Monitoring (2)
- -Ecological Health (5)
- -Advanced Methods for Prediction of Biological Community Dynamics (3)
- Degradation/Transformation of MC and Emerging Contaminants (3)
- -Environmental Risk (7) [2 in Nanomaterials]
- -Plant Interactions (1)
- Archeological Post Depositional Processes (0)
- Impact of Climate Change on Chemical Interactions (1)
- Biologically Inspired Networks as Model for Engineered Systems (3)

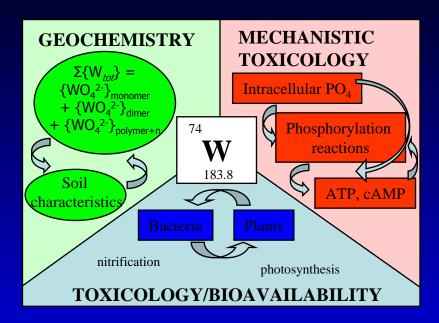


### Risk Related Applied Research and Advanced Development

- Predictive Toxicology for Munitions Constituents (MCs)
- Nanotechnology Development for the Warfighter: Environmental Quantification and Classification
- Computational Chemistry of Explosives: Prediction of Environmental Fate and Toxicity in Water
- Toxicogenomics for Assessment of Munitions Constituents



### Environmental Fate and Toxicity of Tungsten



Schedule & Cost

Schedule & Cost								
Milestones	Prior Yrs	FY06	FY07	FY08	FY09	To Comp.		
ATP in cultered cells		0	1					
Batch Exp. For Kd of tungstate	<b>(</b>		1					
Plant-microbe exposure-response exp in W amended soil		<u> </u>	1	•				
Prelim Geochem Modeling		7	<b>(0)</b>	1				
Plant-microbe exposure- response/uptake exp in field soil			0		1			
Batch and column exp (vs. pH, soil type, PO4)		<b>(</b> 0	· ·	1				
Protein-tyrosine kinase activity in cultured cells		·	0					
Reactive transport simulation				1	•			
Cyclic AMP in cultured cells	_			<b>(0)</b>	(1)			
Report and manuscript preparation						1		

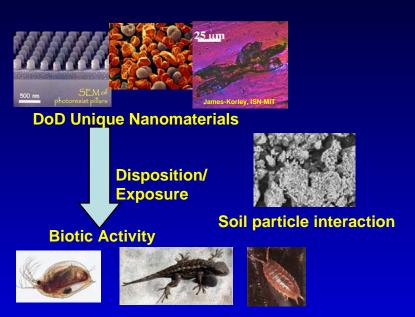
**Purpose:** Determine factors controlling tungsten fate, transport, bioavailability, and its mechanisms of toxic action.

### **Product/Results:**

- Define equilibrium expressions of major tungsten reactions for model input
- Elucidate tungsten toxicity mechanism, specifically effects on intracellular phosphorylation reactions, and critical Mo-based nitrogen cycling enzymes
- Quantify effects of tungsten on nitrogen cycling and photosynthetic processes

- Quantify tungsten fate in training range environment for sustainable operations
- Significant data/mechanisms/mode of action for input to risk assessment models
- Improved assessment of tungsten fate
   Best Management Practices = Range
   Sustainability

# Nanomaterial Structure Influence on Biological Susceptibility



#### Schedule & Cost

	Prior				То
Milestones	Yrs	FY06	FY07	FY08	Comp.
Data gap analysis and conceptual					
model	\				
Interaction of NM w ith soil and		<u> </u>			
w ater		,			
Nature of NM interaction with biota			<		1

### **Purpose:**

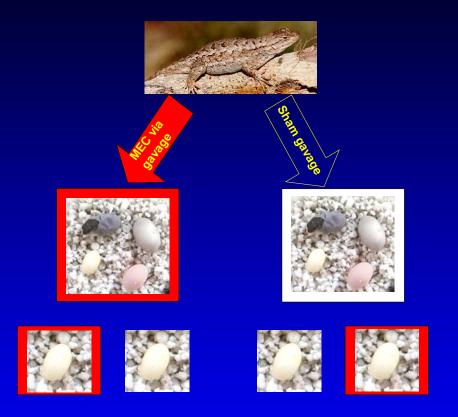
- Investigate the unique properties of DoD relevant engineered nanomaterials (NM; e.g., soldier materials, energetics, obscurants)
- Role of properties in physical, chemical, and biological interactions with the environment.

### **Product/Results:**

- Identify data gaps and develop conceptual model for threats to nanotechnology development.
- Characterize the interactions of selected NM with environmental media and biota.

- Greater understanding of potential environmental transport and biotic activity from implementation of engineered NMs in advanced technologies.
- Significant cost savings from proactive approach for best management of nanotechnology.
- Follow on and leveraging opportunities with many innovative research laboratories (DoE, Industry, Universities) to further investigate unique properties of NMs.

### Exposure pathways for early life stage reptiles



#### Schedule & Cost

Milestones	Prior Yrs	FY07	FY08	FY09	FY10	To Comp.
Uptake of explosives by eggs				1		
Maternal deposition of explosives			< C		1	
Cumulative exposure and bioavailability of explosives				<b>(</b>	1	

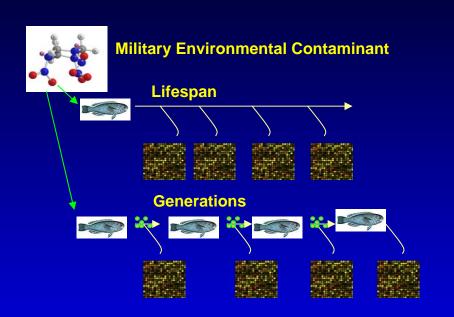
**Purpose:** Explore in ovo exposure of explosives in fence lizards (Sceloporus spp.) and the fraction transferred during egg production by female lizards.

### **Product/Results:**

- Availability of explosives from contaminated nesting substrate in developing lizard eggs.
- Maternal transfer of explosives to lizard eggs following oral exposure.
- Cumulative exposure of maternal transfer and in ovo uptake of explosives.

- Define exposure pathways for reptile ecological receptor used in risk assessments on installations.
- Improved assessment of military impacts on novel ecological receptors = Better Management = Increased Range Access.

# Genomic Evolution & Acclimation: Genomic Response to Long-term and Multigenerational Exposure to Contaminants



**Purpose:** Understand interaction between long-term and multigenerational exposures to contaminant and genomic responses

### **Product/Results:**

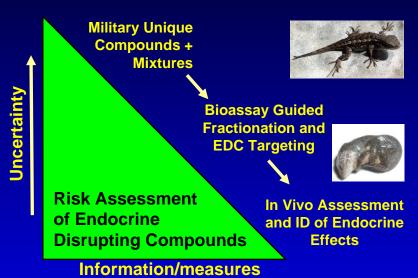
- Experimentally-based assessment of genomic acclimation and dynamics
- Determine roles of mutational and transient adaptation in genomic responses of offspring.
- Impact of chronic RDX exposure on critical behavior, growth, and reproduction

#### Schedule & Cost

	cneau	ie a cc	IST		
Milestones	Prior	FY06	FY07	FY08	То
Wilestolles	Yrs	F100	FIUI	F108	Comp.
Chronic Exposure over lifespan	6		1		
Chronic Exposure over multiple					
generations				1	
Genomic Analysis		0		1	

- Better understanding of what observable genomic patterns indicate relative to exposure to contaminants and impacts
- Key step towards future use of genomics in environmental monitoring and risk assessment
- New information on organismal responses to chronic, multi-generational exposure.

### Do Ordnance Related Compounds Affect the Endocrine System in Reptiles?



Purpose: Investigate the potential for contaminants present at military installations (RDX, HMX, TNT) to cause endocrine mediated reproductive and/or developmental effects in wildlife.

### **Product/Results:**

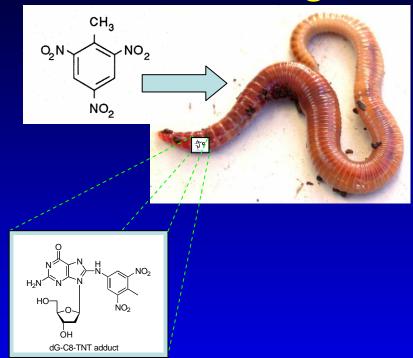
- Reptile model (western fence lizard) for wildlife studies.
- Identification and characterization of endocrine modulating compounds and chemical mixtures.
- Fractionation approach to assess large number of contaminants in a single analysis.

### Payoff:

- Greater understanding of the potential for developmental and reproductive effects and risk resulting from contaminants present at military facilities
- Significant cost savings from assessment of large number of contaminants by using bioassay guided fractionation (BGF).
- Reduce overly-conservative management practices that result from inadequate information.

# Schedule & Cost Prior Yrs FY06 FY07 FY08 Comp. Develop WFL EDC model and BGF BGF analysis using WFL and assay Develop and repro WFL study

# A Sticky Clue to Exposure: Toxicological Understanding and Use of "Bound Residues"



#### Schedule & Cost

	Prior				То
Milestones	Yrs	FY07	FY08	FY09	Comp.
Potential TNT- protein/ DNA			<u></u>		
adducts					
Multi-compartment eval. Of TNT		<b>(</b> 0		1	
bioaccumulation					
Identifiication of bound residues as			<b>(0)</b>	<b>1</b>	
novel biomarkers					

**Purpose:** Provide molecular-level understanding of TNT-'bound-residues' in terrestrial invertebrates and identification of unique markers of exposure.

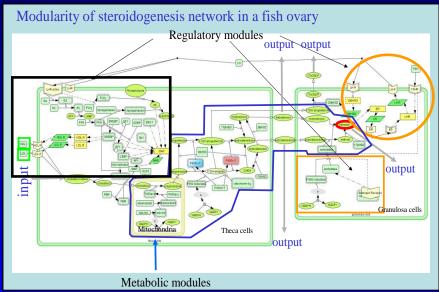
### **Product/Results:**

- Multi-compartment toxicokinetic assessment of TNT bioaccumulation in earthworms.
- Identification and relative abundance of TNT products bound to tissue (i.e., specific biomarker of exposure)

- Improved understanding of biological consequences of soil exposure to MECs
- Identification of novel markers of exposure with long half-lives with potential for development into powerful monitoring tools.
- Improved assessment of military impacts on soil organisms resulting in better management practices.

# The Network Properties of Ovarian Steroidogenesis in a Small Fish





#### Schedule & Cost

	Prior				То
Milestones	Yrs	FY07	FY08	FY09	Comp.
Exposure and microarray analysis	\(\frac{1}{2}\)		1	1	
Reverse Engineering of networks			0	1	
Test robustness and fragility of network			<b>O</b>	1	<b>&gt;</b>

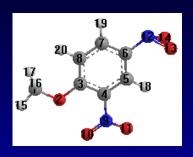
<u>Purpose:</u> Do stressor interactions with fragile points in the steroidogenesis network architecture lead to network failure?

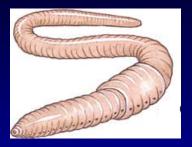
### **Product/Results:**

- Network architecture of steroidogenesis.
- ID of mechanisms controlling network
- Impact of energetics on endocrine function.
- Identification of network points susceptible to chemical attack.

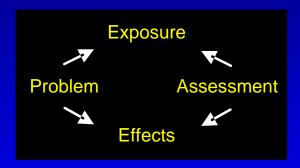
- Characterize relationship of robustness/fragility trade offs in model system.
- Novel model of complex systems.
- Improved understanding of how complex systems function.

### Computational Chemistry and Toxicity of DNAN





### **RISK**



#### Schedule & Cost

Milestones	Prior Yrs	FY08	FY09	FY10	To Comp.
Computational Predicitons of	(				
Phys/Chem Properties	/				
Validation of Computational					
Predictions via Terrestrial		<u> </u>			
Toxicity Evaluation of DNAN and					
Degradation products		<b>(</b> 0		$\sim$	/

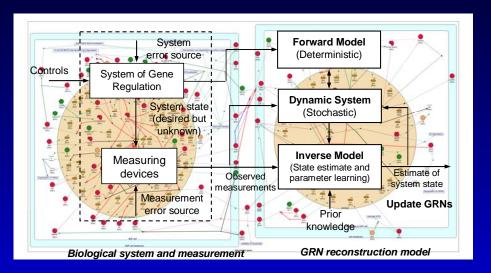
**Purpose:** Investigate the physical and chemical properties of DNAN and evaluating the toxicity of this emerging compound.

### **Product/Results:**

- Structurally, we predict DNAN will act similarly to other nitroaromatics, DNT and DNP.
- Better definition of the interplay between computational chemistry and toxicology as it relates to munitions.

- DNAN present environmental issues as it is released during munitions manufacturing, testing, training and use.
- The approach will be to fill knowledge gaps essential to remediation of health hazards to Army and DoD personnel.

### Development of a Novel Earthworm Neurotransmission Network Model of Sublethal Neurotoxicity



**Purpose:** Understand how interactions among neurotransmission pathways in the networks are affected and recover.

### **Product/Results:**

- A novel GRN connecting major neurotransmission pathways of E. fetida.
- Identification and validation of the gene targets of RDX in E. fetida.
- Elucidation of RDX neurotoxicity mechanisms.

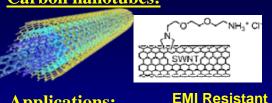
#### Schedule & Cost

	Prior				То
Milestones	Yrs	FY08	FY09	FY10	Comp.
Phase 1: model conception	<u> </u>	1			
Phase 2: model construction		<u> </u>	1		
Phase 3: model validation			\(\frac{\chi}{c}\)	1	

- Fundamental understanding of a biological network.
- The groundwork for systematic and fundamental understanding of neurotoxicology in soil invertebrates.
- Enhance capabilities in environmental risk assessment and predictive risk models.

### Factors Influencing Partitioning / Risk of

### **Carbon nanotubes:**







Stronger / lighter armor





**Model species:** 







#### Schedule & Cost

Milestones	Prior Yrs	FY07	FY08	To Comp.
Particle size toxicity in sediment		0	1	
Partitioning of NT modifications		0	<u> </u>	1
Conduct of novel and relevant bioassays		0		1

#### **Nanotubes** Purpose: Investigate -

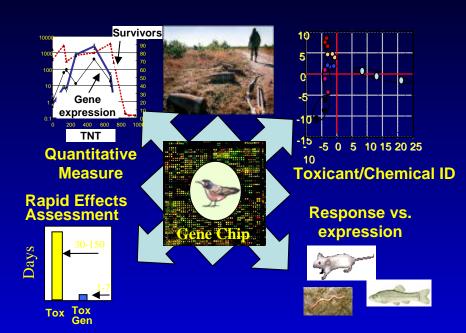
- The fate of NTs
- Alterations due to surface modifications (engineered or naturally occurring)
- Role of particle size and shape
- Toxicological implications

### **Product/Results:**

- Publications / presentations: Data on how surface modifications influence toxicity
- Insight on how to properly conduct biological effects assessments of nanotubes

- Provide research community and Army technology developers with better understanding of the environmental consequences of different NT surface modifications
- Data to assist with green engineering
- Provide the ecotoxicology research community with better methodology for the conduct of biological effects testing
- Feed into the focus area (FY 08 11): Environmental Quantification and Classification of Nanomaterials (Steevens)

### Toxicogenomics for Assessment of Munitions Constituents



#### Schedule & Cost

	Prior				То
Milestones	Yrs	FY08	FY09	FY10	Comp.
Rapic effects assessment with	3				
genomics					
Molecular markers of exposure	2 3				
MC classification by genetic		/2			
response		3			
Molecular mechanics of MC toxicit	2	3			
Similarity of species genomic					
response to MCs	<u> </u>	4	7		
Toxicogenomic Eval. Rapid					
screening/ monitoring of ecological	(3			5	
impact of MCs					

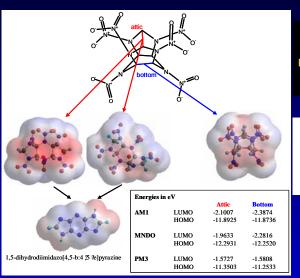
**Purpose:** Provide capability to rapidly screen and accurately monitor the ecological impact of munitions constituents (MCs) using measures of gene expression or toxicogenomics

### Results:

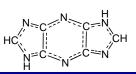
- A toxicogenomic framework to assess sublethal effects.
- Genetic flags to detect exposure.
- Identification of toxicants by genetic fingerprinting
- Prediction of long term impact from short term effects
- Quantitative measure of MC impacts on ecological model species.

- Rapid adverse effect screening
- Biomarkers of MC exposure
- Increased accuracy of ecological impact monitoring
- Significant savings for range managers in monitoring and assessing risk and cleanup levels.
- Follow on and leveraging opportunities new customers and users (Tri-services, EPA, DOE, Industry, as well as other agencies)

### Computational Chemistry of Explosives: Prediction of Environmental Fate and Toxicity in Water







#### Schedule & Cost

	Prior				То
Milestones	Yrs	FY08	FY09	FY10	Comp.
Predictions of chemical structures					
and physical properties of	4				
explosives dissolved in water					
Predictionof reactivity and					
decomposititon of explosives (3				4	<b>&gt;</b>
dissolved in water					
Prediciton of toxicity of explosives					
and their products of 3				4	
decomposition dissolved in water					
Predicition of chemical mechanisms		(3		5	\
of biodegradation and cytotoxicity		\		V	

**Purpose:** Develop new approaches and in silico prediction of physical properties, chemical reactivity and toxicity of explosives dissolved in water, their product of environmental degradation and their metabolites by application of high performance computational chemistry (CC) techniques.

### Results:

- Computational techniques enabling greater throughput and increased rigor in screening of environmental behavior and potential toxicity of current and future explosives.
- New computational protocols providing accurate and computationally inexpensive ways to predict physical properties and rates of explosives decomposition in water.
- Novel <u>QSAR equations correlating toxicity</u> (cytotoxicity) of explosives and products of their degradations with their <u>electronic properties</u> and reactivities in water.

- Significant cost savings from application of CC predictions to estimate risk assessment and toxicological impact of explosives and their metabolites dissolved in water.
- Maximized benefit of costly empirical studies on explosives and their transformations;
- Expedited design and implementation of site management and long-term monitoring projects.

### Nanotechnology Development for the Warfighter: Environmental Quantification and Classification



**Purpose:** Enable the Army's ability to field advanced nano-based technology by appropriate framing of the environmental impacts of nanomaterials.

### **Products:**

- Quantitative approach for multi-dimensional exposure parameters for nanomaterials – integrating surface area, structure, size, and particle density.
- Enhanced periodic table classification system for nanomaterials - physical and biotic.
- Framework for integrating environmental attributes analysis with nanotechnology development decisions.

### Payoff:

- Unencumbered ability to field nanomaterial based warfighting technologies.
- Substantial cost savings from proactive environmental management of nanotechnology.
- Greater understanding of potential environmental transport and biotic activity of nanomaterials.
- Follow on and leveraging opportunities with many innovative research laboratories (DoE, Industry, Universities).

#### Schedule & Cost

Schedule & Cost								
	Prior				То			
Milestones	Yrs	FY08	FY09	FY10	Comp.			
Analytical Structure for								
Characterization	<b>7</b>				7			
Subtask: Tools for Quantifying		<u></u>						
Structure			7					
Subtask: Exposure Quantification	(		4					
Metric	/			<u> </u>				
Subtask: Environmental Reactivity		3		4				
Nanomaterial Periodic Table and	/.			5				
Classification	/							

## Training Range Environmental Evaluation and Characterization System (TREECS)



#### Schedule & Cost

	Prior				То
Milestones	Yrs	FY08	FY09	FY10	Comp.
Automated data input and sourceterm development	<	3	6		
Formulate MC transformation sequestration routines		3	6		
Couple Multi scaler, multi-pathway, multi-media transport with hydraulic models			3	6	
Beta Verification/ Validation				4	6

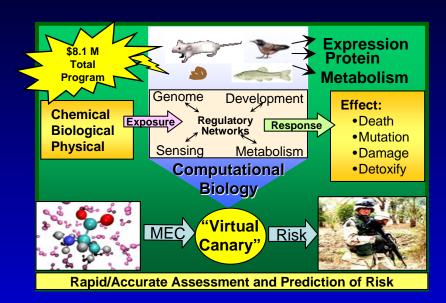
Purpose: Develop an integrated, multi-scale, multimedia, multipathway simulation capability for evaluation of distributed sources of munitions constituents (MC).

### Results:

- Rapid and reliable forensic and predictive assessment of MC migration.
- Quantifiable linkage of range use to future risk of MC migration.
- Risk evaluation capability designed to meet Army needs for proactive land management.

- Ranges operated as a sustainable resource.
- Avoidance of range down time due to EQ constraints.
- Cost avoidance associated with range management vis costly remedial action.

# Predictive Toxicology for Munitions Constituents (MCs)



#### Schedule & Cost

	Prior				То			
Milestones	Yrs	FY08	FY09	FY10	Comp.			
Mathematical modeling of toxicity								
and effects due to existing, well			3	4	$\rightarrow$			
characterized MC								
Multiple stressor impacts on		/.		3				
toxicity		\		2				
MC toxicity mechanisms in		<u>/.</u>	3					
ecological species		/	2/		4/			
Developmental pathways affected		/.						
by MCs		(	3		4			
Cross species validation of MC			/.		-			
effects			(	7	5			
Predictive toxicology computaional			/		6			
biology tool			\ <u>'</u>		, o			

<u>Purpose:</u> Provide capability to predict the ecological toxicity of new and existing MECs.

### Results:

- A toxicogenomic and computational biology tool to predict potential toxic effects of MECs
  - AKA Computational "Canary in a Coal Mine".
- Rapid, quantitative assessment of toxicity of poorly characterized MECs in ecological species.
- Minimized uncertainty = realistic cleanup levels.

- Increased range safety.
- Cost savings by reduced range down time.
- Reduced environmental impact
- Increased range sustainability
- Increased soldier safety

### Microbial Ecology and Geochemistry of Iraqi Airborne Dust



Schedule & Cost

Somedate a Cost						
	Prior				То	
Milestones	Yrs	FY06	FY07	FY08	Comp.	
Sample collection and physical	(		1			
charac.	/	<u></u>	\ <u>'</u>			
Microbiological and geochemical						
charac.						
Correlate physical and						
biogeochemical charac. And			<b>(0)</b>			
behavior			<b>V</b>			

**Purpose:** Determine if airborne dust in Iraq differs from dust of U. S. desert conflict area analogues in it's potential to produce environmental risk

### **Product/Results:**

- Comprehensive biogeochemical characterization of Iraqi dust in context of environmental and human health risk
- Physical behavior of dust particles with respect to biogeochemical fate under ambient and physiological conditions

- Fill basic knowledge gaps regarding the microbial ecology, geochemistry and mineralogy of desert top soils
- Bridge knowledge gap between conflict area analogues and Gulf Region for operational behavior of troops/equipment

