



Nanotechnology-inspired Grand Challenges in the United States

Mike Roco
NSF and NNI

US-Korea Nano Forum, Seoul, September 26, 2016

Nanotechnology-inspired grand challenges

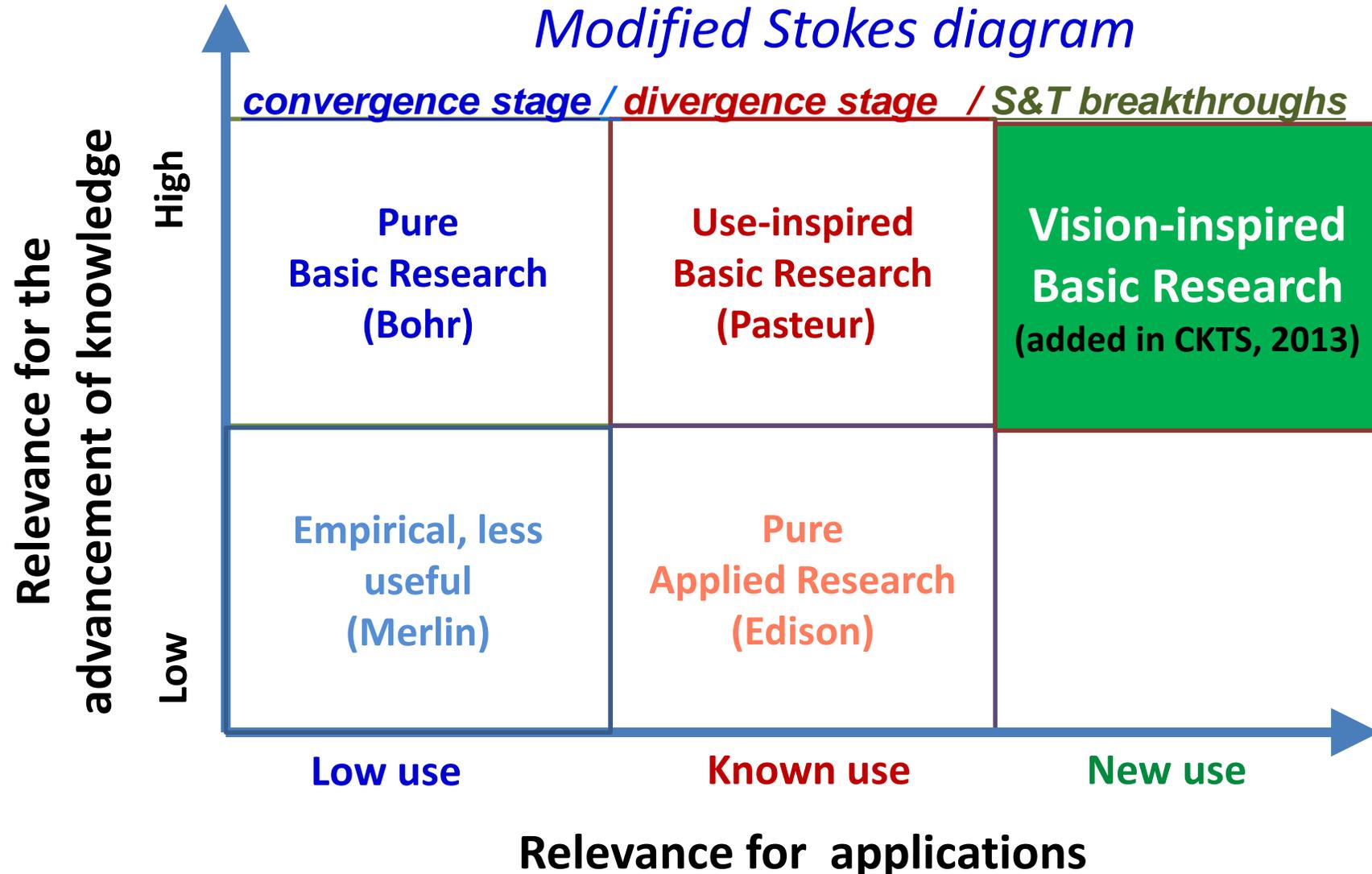
- ✓ S&T breakthroughs, the long-term vision-inspired research, and convergence processes create opportunities for progress
- ✓ Several U.S. priorities in 2016
 - Nanotechnology Signature Initiatives*
 - Nanotechnology-inspired Brain-like Computing*
 - Brain Research*
 - National Strategic Computing Initiative*
 - Food-Energy-Water Systems*
 - National Network for Manufacturing Innovation*

S&T breakthroughs underpin Grand Challenges

(examples of novel concepts targeted by NNI in 2000 "in 20-30 years")

- **Library of Congress in a "one cubic cm" memory device:** target 30-40 atoms (2000); Realized 12-atom structure (IBM, 2012), DNA structure (Harvard, 2012; in "one cubic mm"). *"Millions times smaller"*
- **Exploit nano-photonics:** change direction and frequency of light (2004, then succession of solutions). *"New phenomena and devices"*
- **Molecular cancer detection and treatment** (first gold-shells, Rice, 2002 - 2016 many other solutions in progress) *"Not possible before"*
- **Quasi-frictionless nanocomponents:** quantum fluctuations between selected material surfaces (first Harvard, 2008). *"Almost frictionless"*
- **Magnetic computing** close to the lowest Landauer fundamental limit of energy dissipation under the laws of thermodynamics (STC Berkeley, 2016). *"Millions times less energy consumption"*

Vision-inspired discovery and inventions are essential for the future of innovation



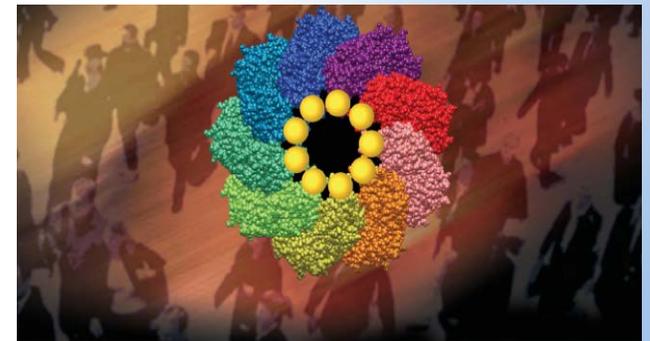


Defining S&T convergence

Convergence is deep integration of knowledge, tools and other relevant areas of human activity that enable each other

- to allow society to answer questions, resolve problems and add-value that isolated capabilities cannot (*is goal oriented*),
- as well as to create new ideas, competencies, technologies, and products on that basis

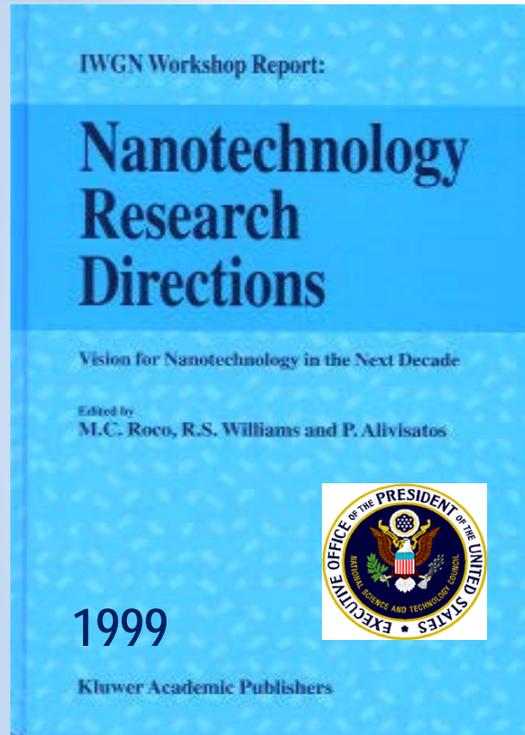
(divergence stage; see ~20 new NNI domains such as: plasmonics, metamaterials, modular DNA NT, nanofluidics, carbon electronics, nano-wood fibers, ...)



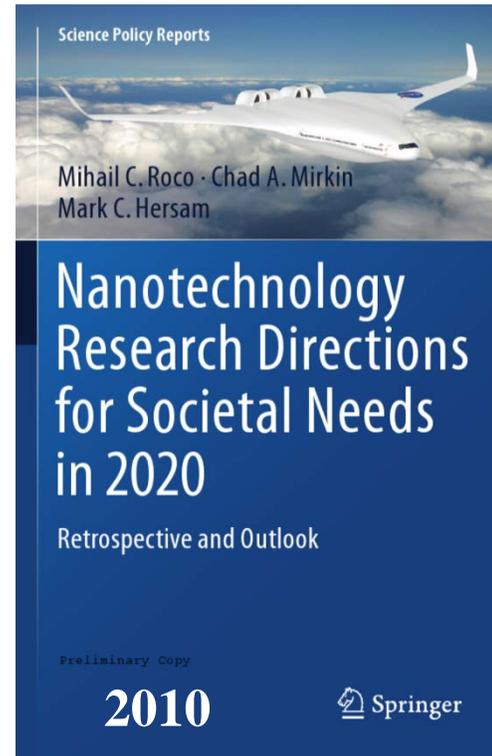
- changing the system by using six convergence principles

Nanotechnology: from scientific curiosity to immersion in socioeconomic projects

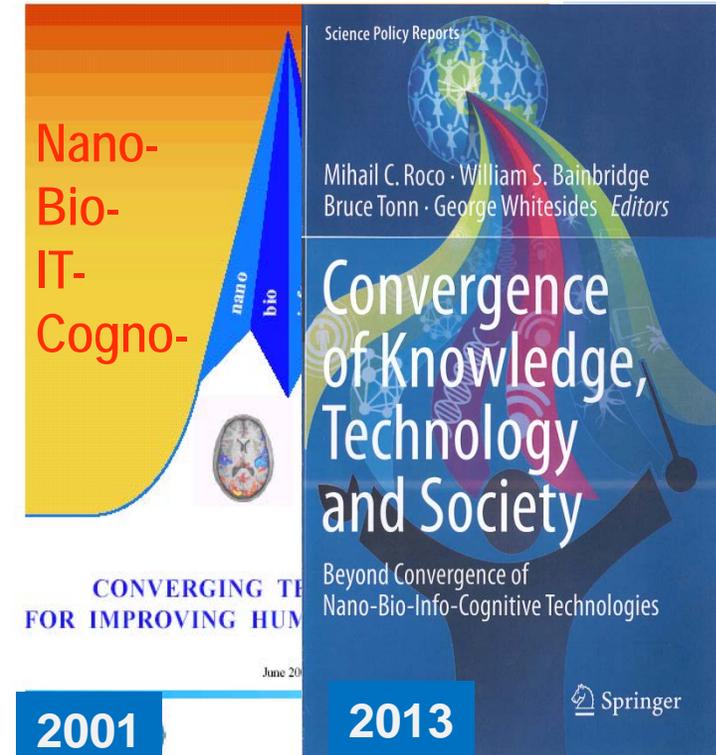
nano1 (2001-2010)



nano2 (2011-2020)



NBIC1 & 2 (2011-2030)



30 year vision to establish nanotechnology:
In 3 stages changing focus and priorities

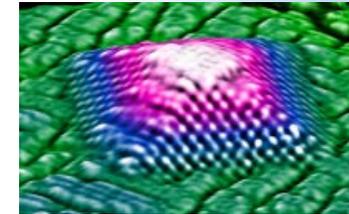
Reports on: www.nano.gov (NNI), www.wtec.org/nano2/ and www.wtec.org/NBIC2-report/ (Refs. 2-5)



Three stages of convergence

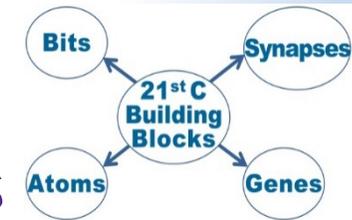
I. Nanoscale Science, Engineering and Technology "Nanotechnology"

Integrates disciplines and knowledge of matter from the nanoscale



II. Nano-Bio-Info-Cognitive Converging Technologies "NBIC"

Integrates foundational, emerging technologies from basic elements using similar system architectures



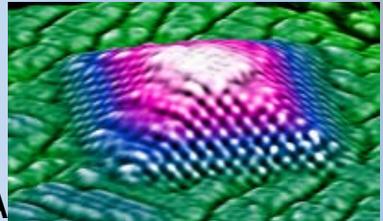
III. Convergence of Knowledge, Technology and Society "CKTS"

Integrates the essential platforms of human activity using six convergence principles

(Ref 5: CKTS Report, 2013)



I. Nanotechnology Convergence leads to R&D programs in 27 agencies



OSTP



Nanotechnology
www.nano.gov

S,T&I convergence-divergence: U.S. National Nanotechnology Initiative, 2000-2030

National Nanotechnology Initiative, 2016
Nanotechnology Signature Initiatives

Sustainable Nanomanufacturing

www.nano.gov/NSINanomanufacturing

Nanoelectronics for 2020 and Beyond

www.nano.gov/NSINanoelectronics

Water Sustainability through Nanotechnology

www.nano.gov/node/1577

Nanotechnology Knowledge Infrastructure

www.nano.gov/NKIPortal

Nanotechnology for Sensors

www.nano.gov/SensorsNSIPortal

Other considered topics are related to: nanomodular systems, nanomedicine, nanocellulose, nanophotonics, nano for infrastructure, nano-city

United States - Korea collaboration in 2D materials after the 2015 Forum: NSF award supplements ("2-DARE", 2016)

- "Crystalline Atomically Thin Layers for Photonic Applications".
Humberto Terrones (RPI) (NSF 1648899/ 1433311)
- "Functionalized Monolayer Heterostructures for Biosensors with Optical Readout".
Alan T Johnson, U Penn (NSF 1648869/ 1542879)
- "Scalable Growth and Fabrication of Anti-Ambipolar Heterojunction Devices".
Lincoln Lauhon, NWU U. (NSF – 1648954/ 1542879)
- "Few-Layer and Thin-Film Black Phosphorus for Photonic Applications".
Fegnian Xia, Yale U. (NSF – 1644859/ 1542815)
- "Phosphorene, an Unexplored 2D High-mobility Semiconductor".
Peide Ye, Purdue U. (NSF 1644785/ 1433459)

2014-2017 NSF Awards: Two-dimensional atomic thick materials

NSF award	PI Last Name	Title	Institute
1433311	Terrones	Design, Synthesis, and Device Fabrication of Transition Metal Dichalcogenides for Active and Nonlinear Photonics	Rensselaer Polytech Inst
1433510	Lauhon	EFRI 2-DARE: Scalable Growth and Fabrication of Anti-Ambipolar Heterojunction Devices	Northwestern University
1433541	Huang	Scalable Synthesis of 2D Layered Materials for Large Area Flexible Thin Film Electronics	U of Cal Los Angeles
1433378	Redwing	2D Crystals Formed by Activated Atomic Layer Deposition	PA St U University Park
1433395	Balandin	Novel Switching Phenomena in Atomic MX ₂ Heterostructures for Multifunctional Applications	U of Cal Riverside
1433467	Goldberger	Enhancing Thermal and Electronic properties in Epitaxial Si/Ge/Sn Graphene Heterostructures	Ohio State University
1433307	Robinson	Ultra-Low Power, Collective-State Device Technology Based on Electron Correlation in Two-Dimensional Atomic Layers	PA St U University Park
1433496	Cobden	Spin-Valley Coupling for Photonic and Spintronic Devices	U of Washington
1433490	Xing	Monolayer Heterostructures: Epitaxy to Beyond-CMOS Devices	University of Notre Dame
1433459	Ye	Phosphorene, an Unexplored 2D High-mobility Semiconductor	Purdue University

2015-2018 NSF Awards: Two-dimensional atomic thick materials

NSF award	PI Last Name	Title	Institute
1542883	Pop	Energy Efficient Electronics with Atomic Layers (E3AL)	Stanford U
1542741	Zhang	Valley Optoelectronics with Atomically Thin MX2	UC Berkeley
1542807	Kim	Quantum optoelectronics, magnetoelectronics and plasmonics in 2-dimensional materials heterostructures	Harvard U
1542864	Salehi-Khojin	Thermal Transport in 2D Materials for Next Generation Nanoelectronics-From Fundamentals to Devices	U of Illinois Chicago
1542863	Menon	Excitonics and Polaritonics using 2D materials (ExPo2D)	CUNY City College
1542815	Xia	Few-layer and Thin-film Black Phosphorus for Photonic Applications	Yale U
1542707	Drndic	Two-dimensional nanopores with electro-optical control for next generation biotechnological applications	U of Pennsylvania
1542879	Johnson	Functionalized Monolayer Heterostructures for Biosensors with Optical Readout	U of Pennsylvania
1542747	Li	From Atoms to Devices: Pathways to Atomic Layer Optoelectronics via Multi-Scale Imaging and Spectroscopy	U of Texas Austin
1542798	Wu	Engineering novel topological interface states in 2D chalcogenide heterostructures	Rutgers U New Brunswick

National Science Foundation

National Nanotechnology Coordinated Infrastructure (NNCI)

<http://www.nnci.net/>; 2015-2025; Coordinating office at GA Tech

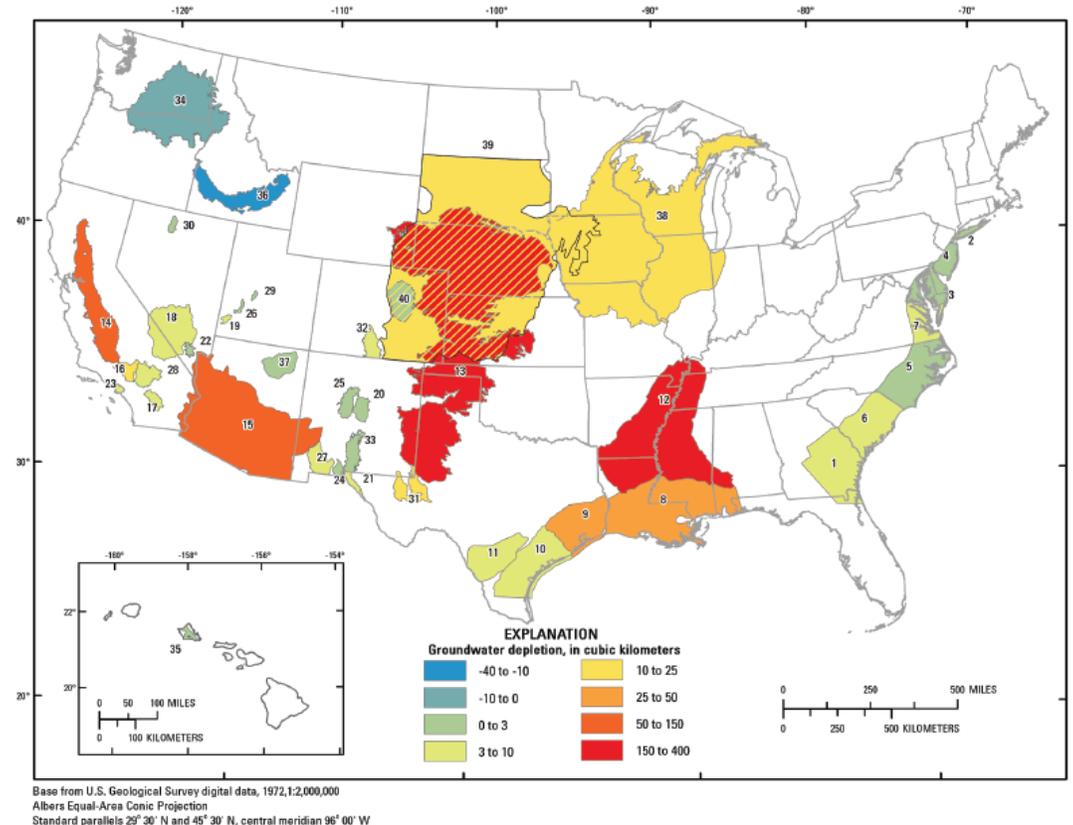


Water Sustainability through Nanotechnology

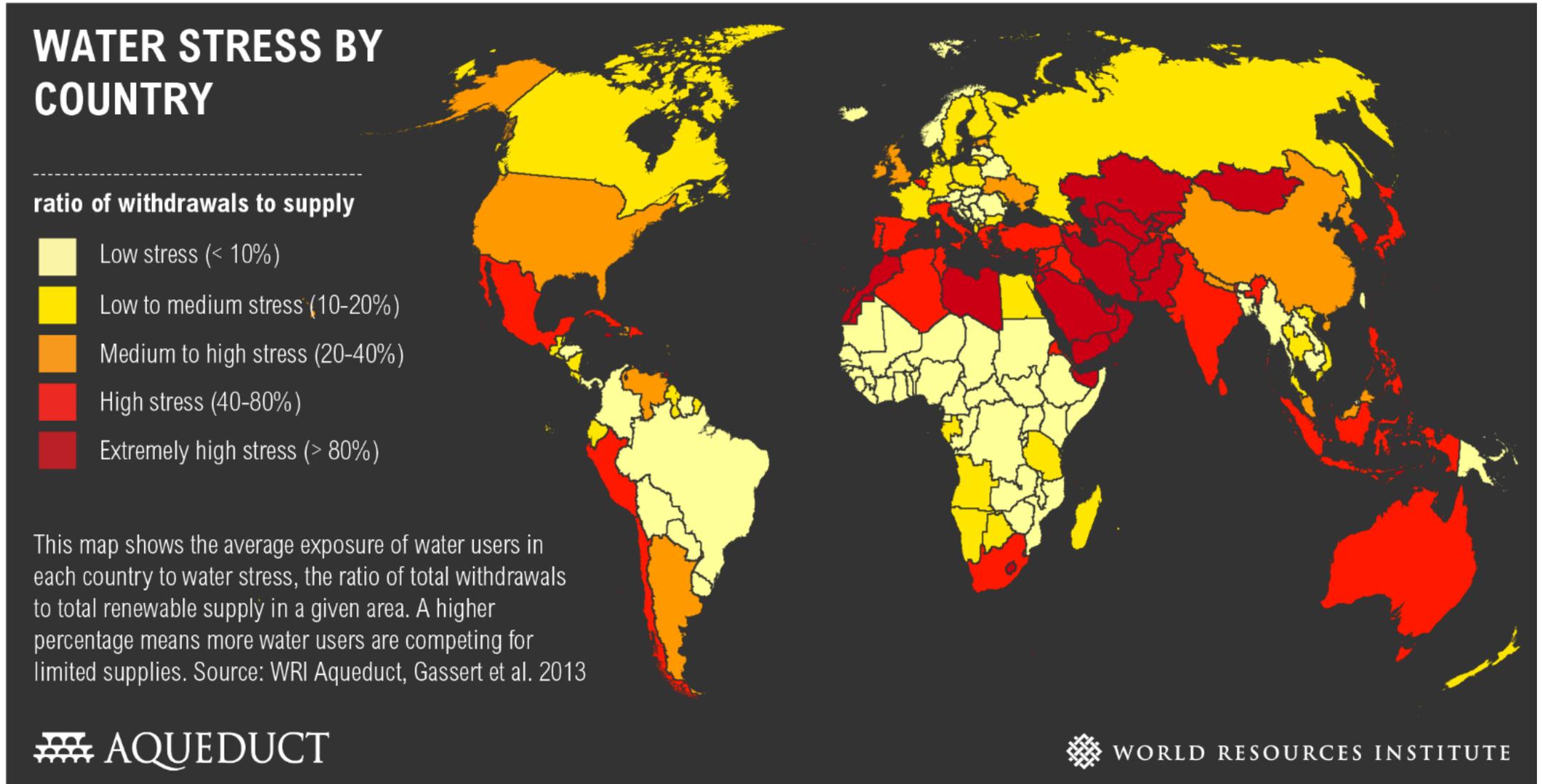
Nanoscale solutions for a global-scale challenge

Research thrusts

- **Increase water availability using NT**
(ex: double the throughput systems within 5 years)
- **Improve the efficiency of water and use with NT**
(Ex: Develop within 5 years nanotechnology-enabled coatings that reduce by 50% the amount of energy)
- **Enable the next-generation water monitoring systems with nanotechnology**
(Ex: continuous, real-time measurement of water quality that are more sensitive, more reliable, easier to use sensors)



Water deficit worldwide



"Brain like computing" (Nano-inspired Grand Challenge)

combining National Nanotechnology Initiative (NNI),
National Strategic Computing Initiative (NSCI) & BRAIN Initiative

- *Nanotechnology-Inspired Grand Challenge for Future Computing* (DOD, DARPA, DOE, IARPA, NSF), announced on Oct 21, 2015:
<http://www.nano.gov/futurecomputing>
- Purpose: "Create a new type of computer that can proactively interpret and learn from data, solve unfamiliar problems using what it has learned, and operate with the energy efficiency of the human brain."

Also: pattern recognition, human like simultaneous perception of information from various sources including the five senses,



Intelligent cognitive assistants (ICA)

May 2016 workshop goals (planned by NSF, SIA, SRC)

- Systems that are highly useful to humans, specifically on the topic of Harnessing Machine Intelligence to Augment Human Cognition and Human Problem-Solving Capabilities – e.g., research that drives towards “Intelligent Cognitive Assistants”
- Explore scenarios for developing the novel architectures, concepts and algorithms which will be required for “assistants” to energy-efficient perceive, compute, and interact, and in this way to provide actionable information and informed advice to their human users.
- Establish a long-term vision (10-20 years), from “knowledge and data” in 2015 to “intelligence and cognition” in 2030



Nanoelectronics Research Initiative Funded Universities (SIA, NSF, NIST)

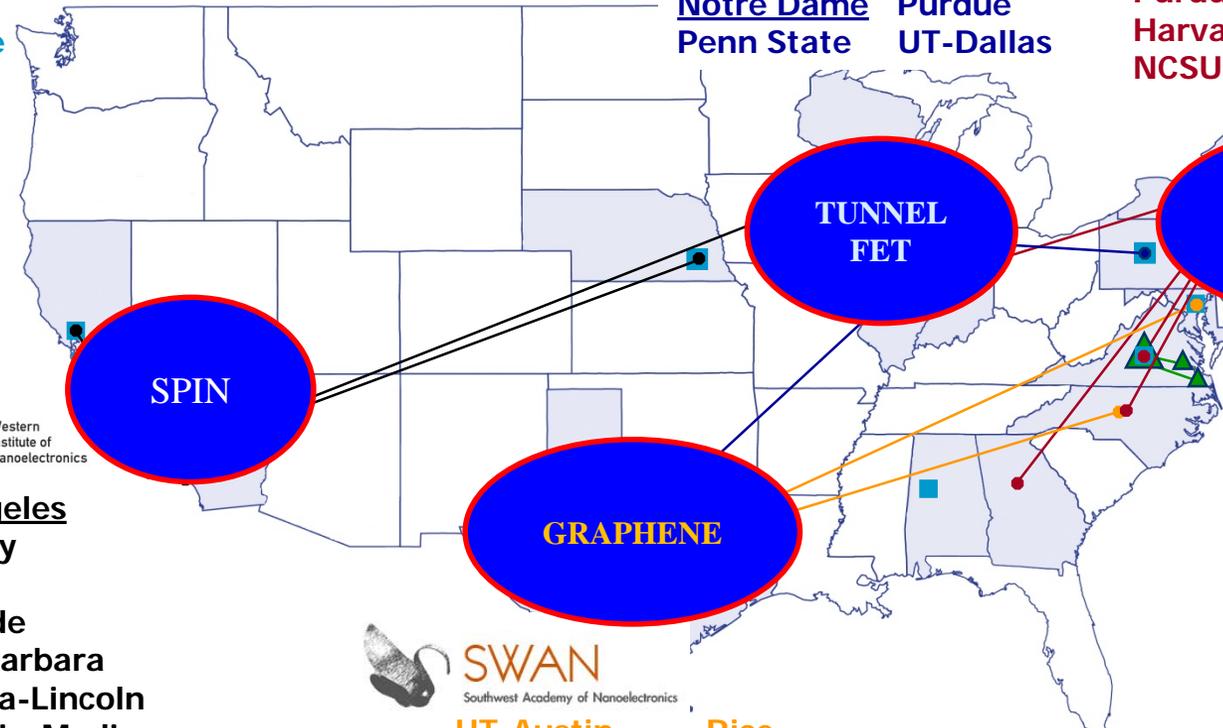


NIST
(co-funds NRI centers)

Nanoelectronics • Architectures
MIND
MIDWEST INSTITUTE FOR NANO-ELECTRONICS DISCOVERY



❖ Awards made in 2011 for collaborative group research (NRI Signature Initiative)



Notre Dame Purdue
Penn State UT-Dallas

SUNY-Albany
Purdue MIT Columbia
Harvard GIT U. Virginia
NCSU

WIN Western Institute of Nanoelectronics

UC Los Angeles
UC Berkeley
UC Irvine
UC Riverside
UC Santa Barbara
U. Nebraska-Lincoln
U. Wisconsin-Madison

SWAN
Southwest Academy of Nanoelectronics

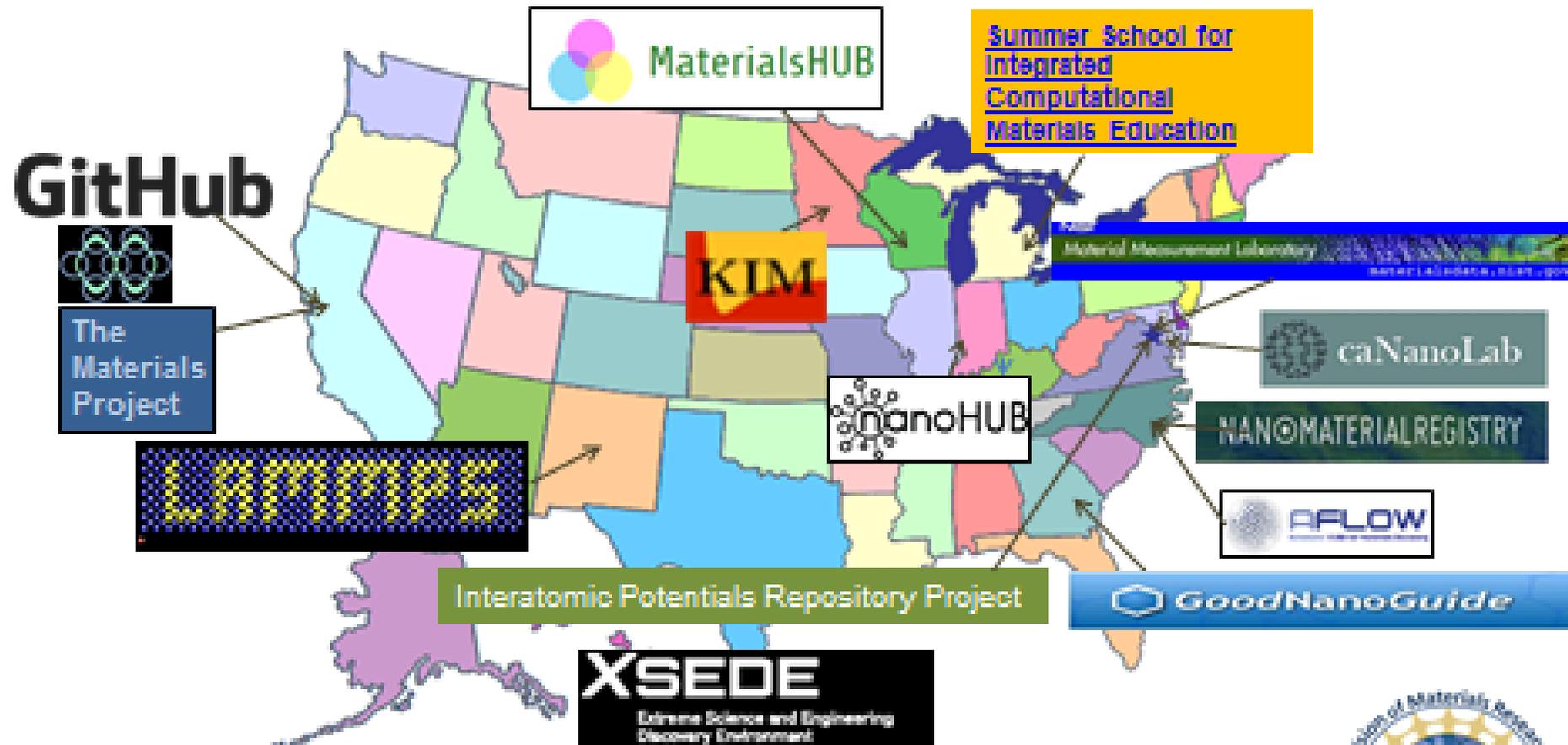
UT-Austin Rice
UT-Dallas Texas A&M
U. Maryland NCSU

■ Brown
Columbia
Illinois-UC
MIT/U. Virginia
Nebraska-Lincoln
Northwestern
Penn State
Princeton / UT-Austin
Purdue
Stanford
U. Alabama
UC Berkeley

▲ Virginia Nanoelectronics Center (ViNC)
University of Virginia
Old Dominion University
College of William & Mary

Partnerships NSF, NIST, SIA, SRC with > 30 Universities in 20 States (2014 -)

Key components of the Nanotechnology Knowledge Infrastructure



- Supported by NIH, NIOSH, NIST, NSF, ONR, DOE

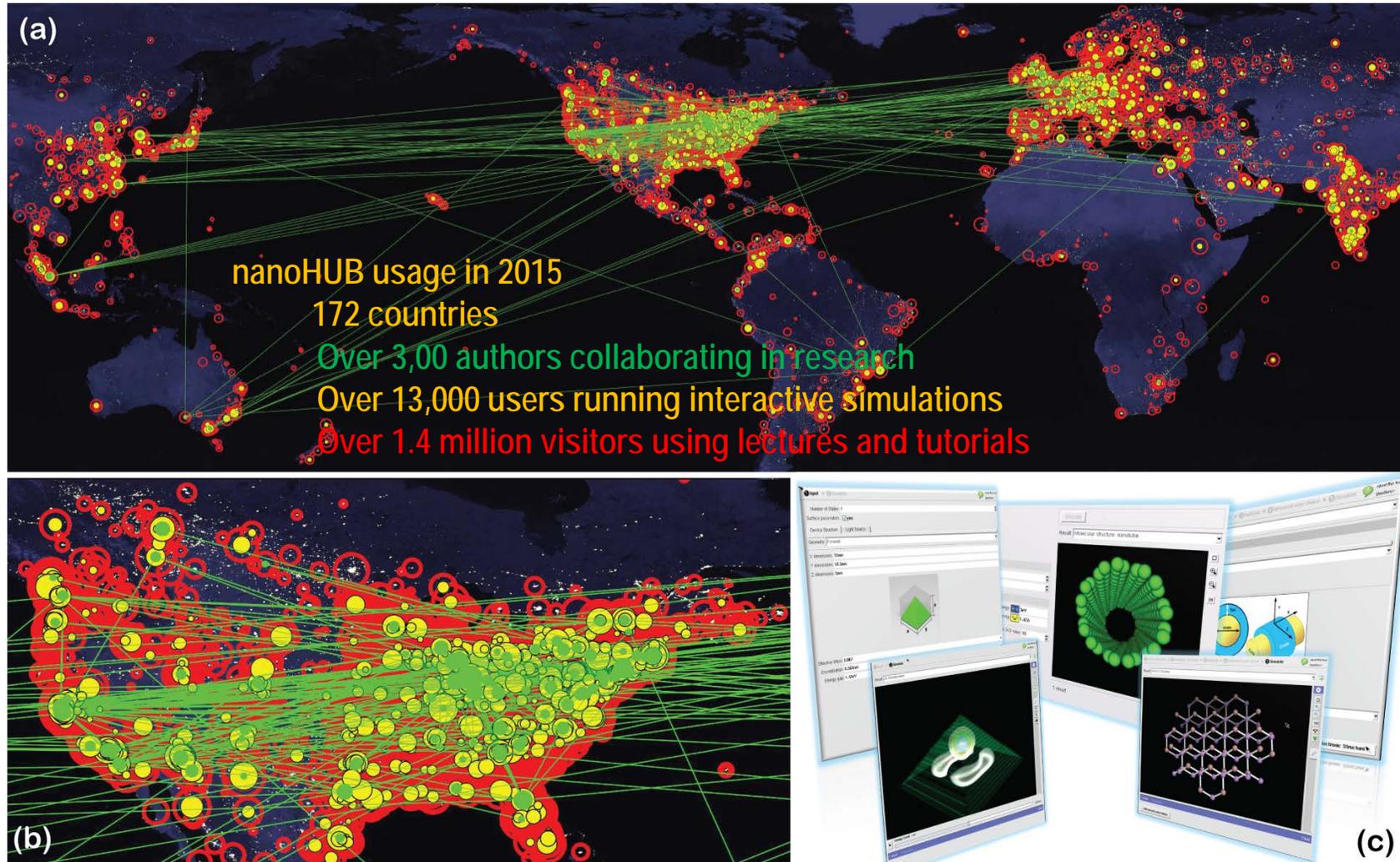
<http://nanoinformatics.org/2015/agenda/>





Network for Computational Nanotechnology (NCN)

nanoHUB.org



(a,b) - Red circles designate visitors viewing lectures, tutorials, or homework assignments.
Yellow dots are users of simulation. Green dots indicate > 1,500 scientific publications citing nanoHUB;
(c) a typical nanoHUB interactive session



UC CEIN Predictive Toxicological Platforms (Andre Nel, 2016)

Nanomaterial libraries

Compositions
metals, metal oxides, CNTs, graphene, silica, quantum dots, etc

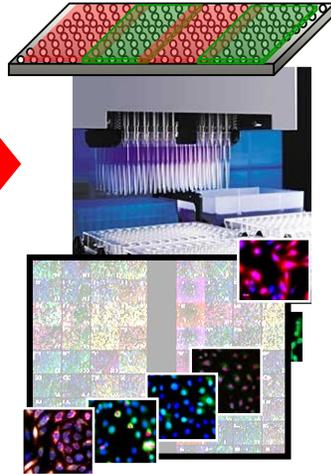
Combinatorial properties
size, shape, aspect ratio, dissolution, band gap, charge, functionalities, coatings etc

New Commercial nanoproducts
profiled against a grid of library materials or data repository

Tiered hazard/risk assessment and exposure-based decision analysis for:

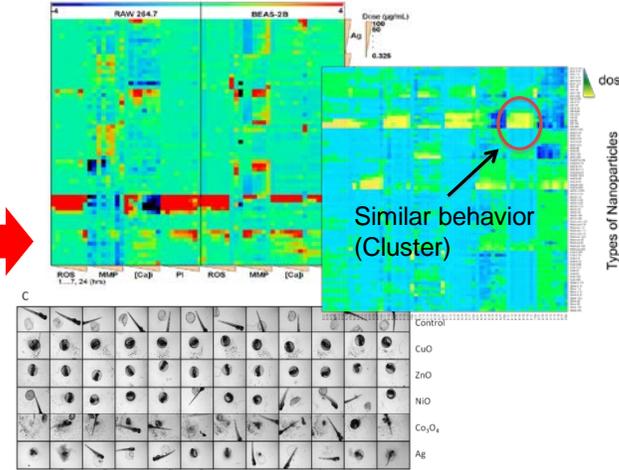
- Safe implementation
- Regulatory decisions
- Reduced animal use
- Reduced Tier 3 testing
- Establishing exposure limits
- Structure-activity analysis
- Safer design

High throughput screening (adverse outcome pathway or AOP based)



Cells, bacteria, yeasts, zebrafish embryos

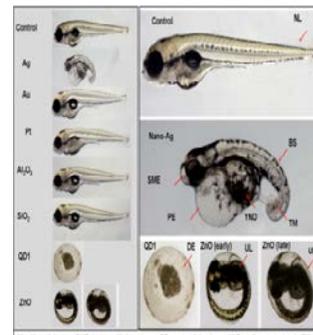
Computational ranking/modeling/predictions



Tier 1
Compare
Rank
Prioritize

Rapid
High volume

Tier 2
Select animal & organism testing (short-terms protocols that reflect the In vitro AOP)

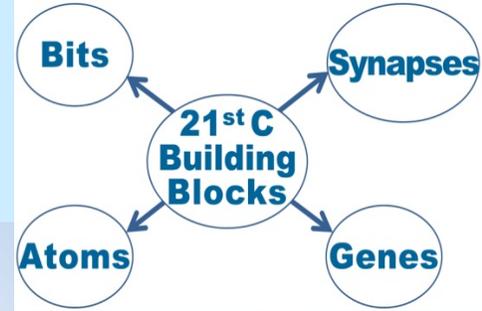


In vivo hazard ranking and prediction testing



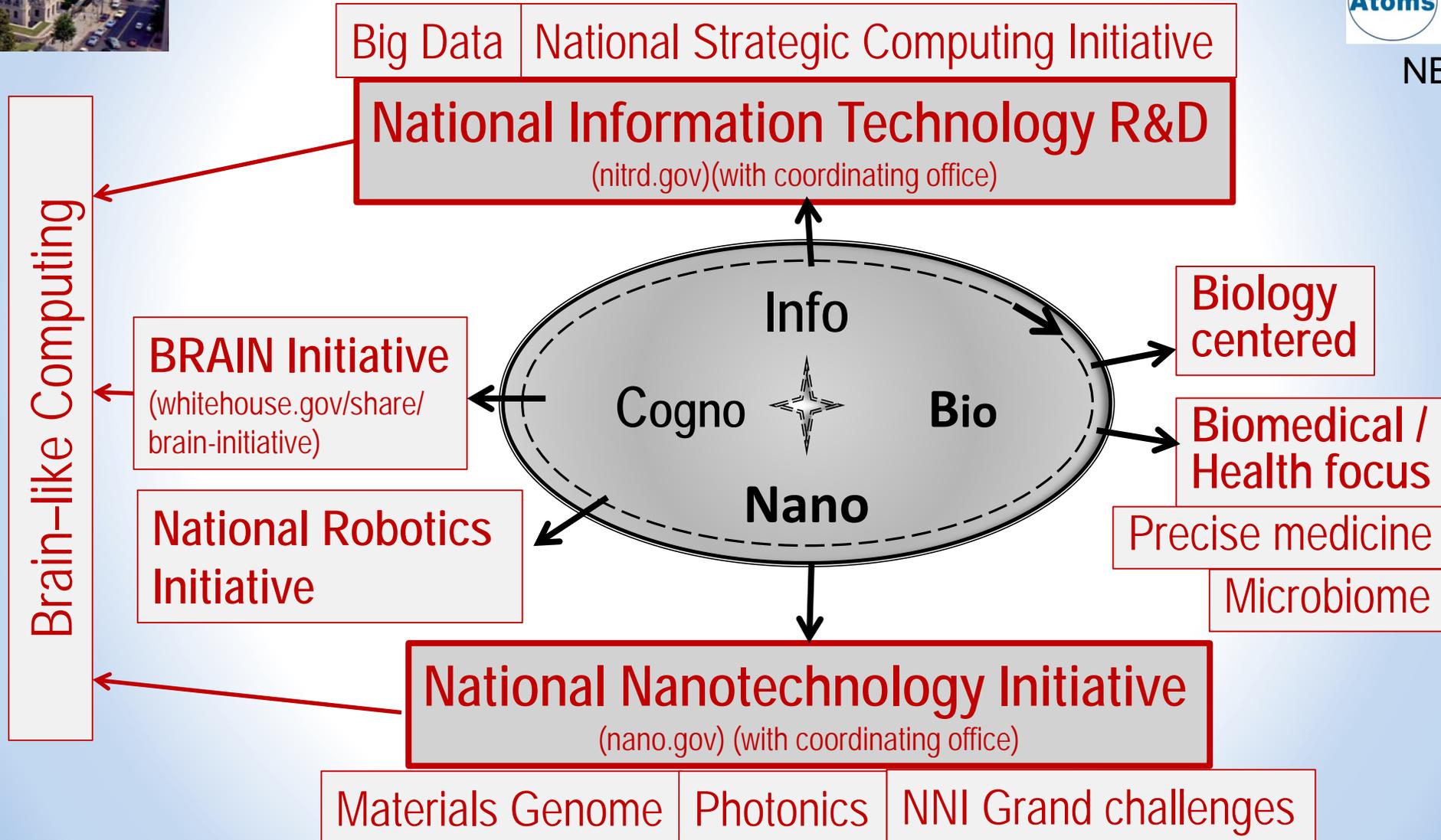
Converging foundational technologies (NBIC) leads to

II. U.S. emerging S&T initiatives



NBIC architecture

OSTP

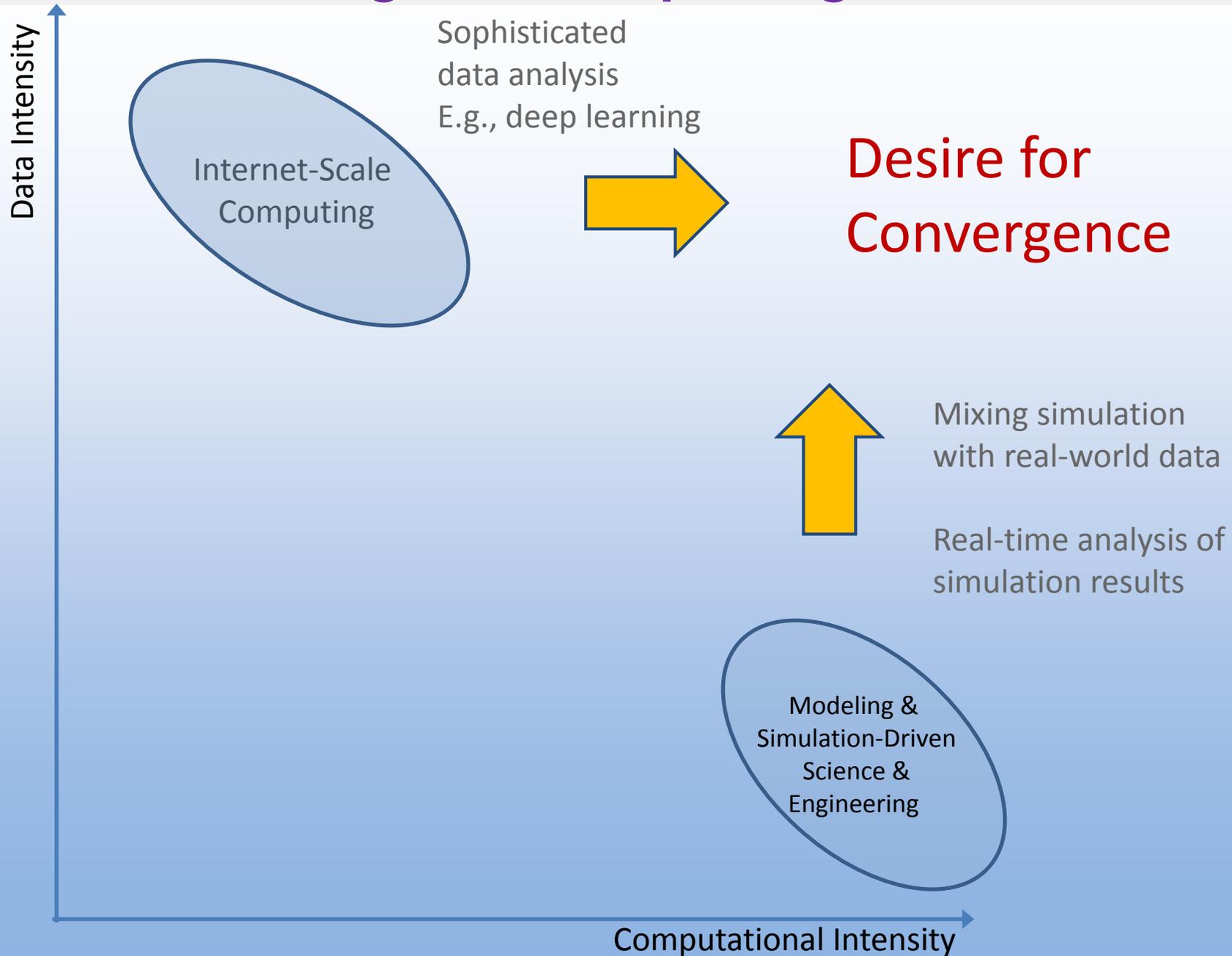


Networking and Information Technology R&D (NITRD) program with 12 research priorities

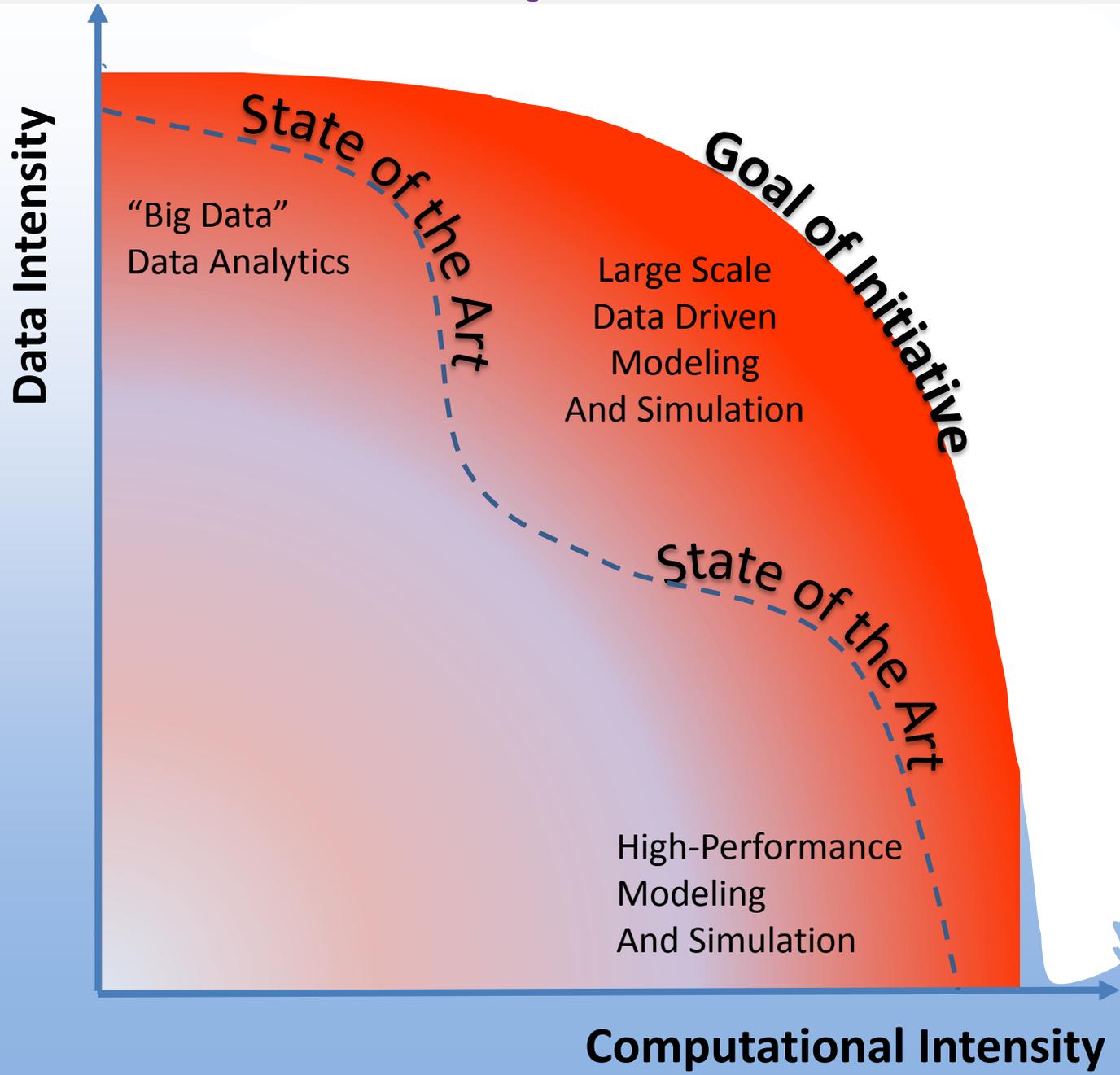
<https://www.nitrd.gov/>

- Big Data (BD)
- Cyber Physical Systems (CPS)
- Cyber Security and Information Assurance (CSIA)
- Health Information Technology Research and Development (Health IT R&D)
- Human Computer Interaction and Information Management (HCI&IM)
- High Confidence Software and Systems (HCSS)
- High End Computing (HEC)
- Large Scale Networking (LSN)
- Software Design and Productivity (SDP)
- Social, Econ., and Workforce Impl. of IT and IT Workforce Develop. (SEW)
- Video and Image Analytics (VIA)
- Wireless Spectrum Research and Development (WSRD)

Convergent Computing Trends



Aspirations for convergence





National Strategic Computing Initiative NSCI

Objectives

1. Accelerate delivery of a capable exascale computing system (hardware, software) to deliver approximately 100X the performance of current 10PF systems across a range of applications
2. Increase coherence between technology base used for modeling and simulation and that used for data analytic computing.
3. Establish, over the next 15 years, a viable path forward for future HPC systems in the post Moore's Law ...
4. Increase the capacity and capability of an enduring national HPC ecosystem, employing ... networking, workflow, downward scaling, foundational algorithms and software, and workforce development.
5. Develop an enduring public-private partnership to assure that the benefits .. are transferred to the U.S. commercial, government, and academic sectors





Rebooting the IT Revolution

2015 SIA & SRC workshop report *sponsored by NSF, NIST and DARPA*

Recommendations (*with research initiatives in 2016*):

- ***Insight technologies ecosystem***. Insight computing requires research in machine learning, data analytics, neuromorphic computing, quantum communication, new approaches for user-machine interfaces, as well as increase computer capacity.
- Data-producing systems increasingly will involve small, low-power sensors and actuators embedded in the physical world—**a network of *sensor-enabled cyber-physical systems within IoT***
- ***Energy-efficient sensing and computing***
- ***Real-time communication ecosystem***
- ***Brain-Inspired Computing***
- ***Multi-level and scalable security***; cybersecurity in manufacturing
- ***Next-generation manufacturing paradigm***



NNI & NITRD: Energy Efficient Computing - from Devices to Architectures (E2CDA)

NSF Workshop for Energy Efficient Computing, April 14-15, 2015

<https://www.src.org/nri/energy-efficient-computing-workshop.pdf>

- Disruptive system architectures, circuit microarchitectures, and attendant interconnect technology aimed at achieving the highest level of computational energy efficiency for general purpose computing systems
- Revolutionary device concepts and associated circuits and architectures that will greatly extend the practical engineering limits of energy efficient computation

Topics aligned with:

- Nanotechnology-inspired Grand Challenge for Future Computing, OSTP 2015
- National Strategic Computing Initiative (NSCI) (OSTP, 2015)

Quantum information systems

- US Interagency Program: **Quantum Information Systems**; in NSF six divisions from MPS, ENG and CISE contribute
- NSF16-502, EFRI, 2016: "**Advancing Communication Quantum Information Research in Engineering (ACQUIRE)**";
"**New Light and Acoustic Wave Propagation: Breaking Reciprocity and Time-Reversal Symmetry (NewLAW)**"
- Research activities in industry (ex. at **IBM Watson Lab.** and government laboratories (ex. at **Sandia National Laboratory**)
- STC on **Integrated Quantum Materials**, Harvard U.; and STC on **Energy Efficient Electronics Science** , UC Berkeley

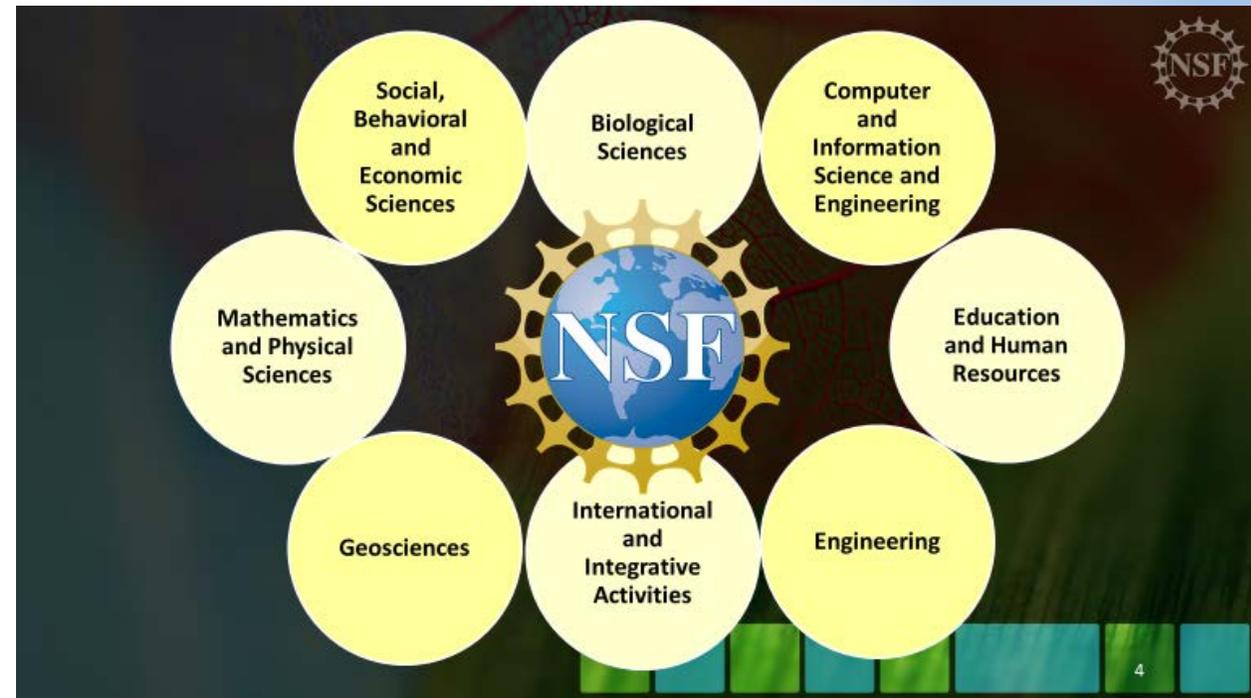
Note: "**Quantum Manifesto**" in EU, an initiative by European science, industry and policy communities, Oct. 2015 call, for a European strategy

BRAIN Initiative

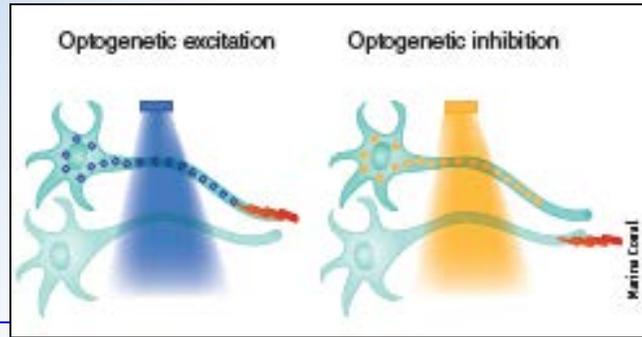


- Federal agencies: NSF, NIH, DARPA, FDA
- Private partners: Allen Institute for Brain Science, Howard Hughes Medical Institute, Kavli Foundation

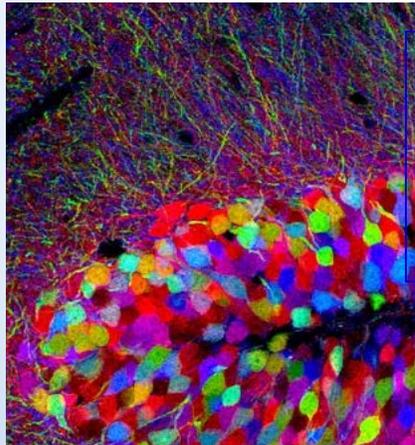
NSF



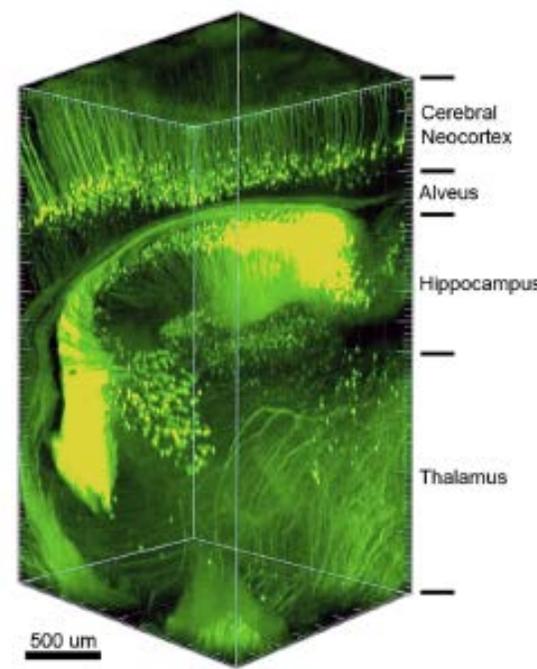
New Tools for Understanding the BRAIN



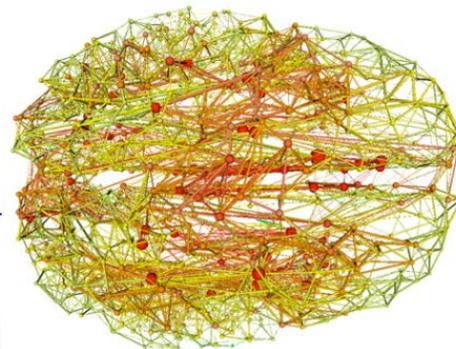
Optogenetic Manipulation



High Resolution Imaging



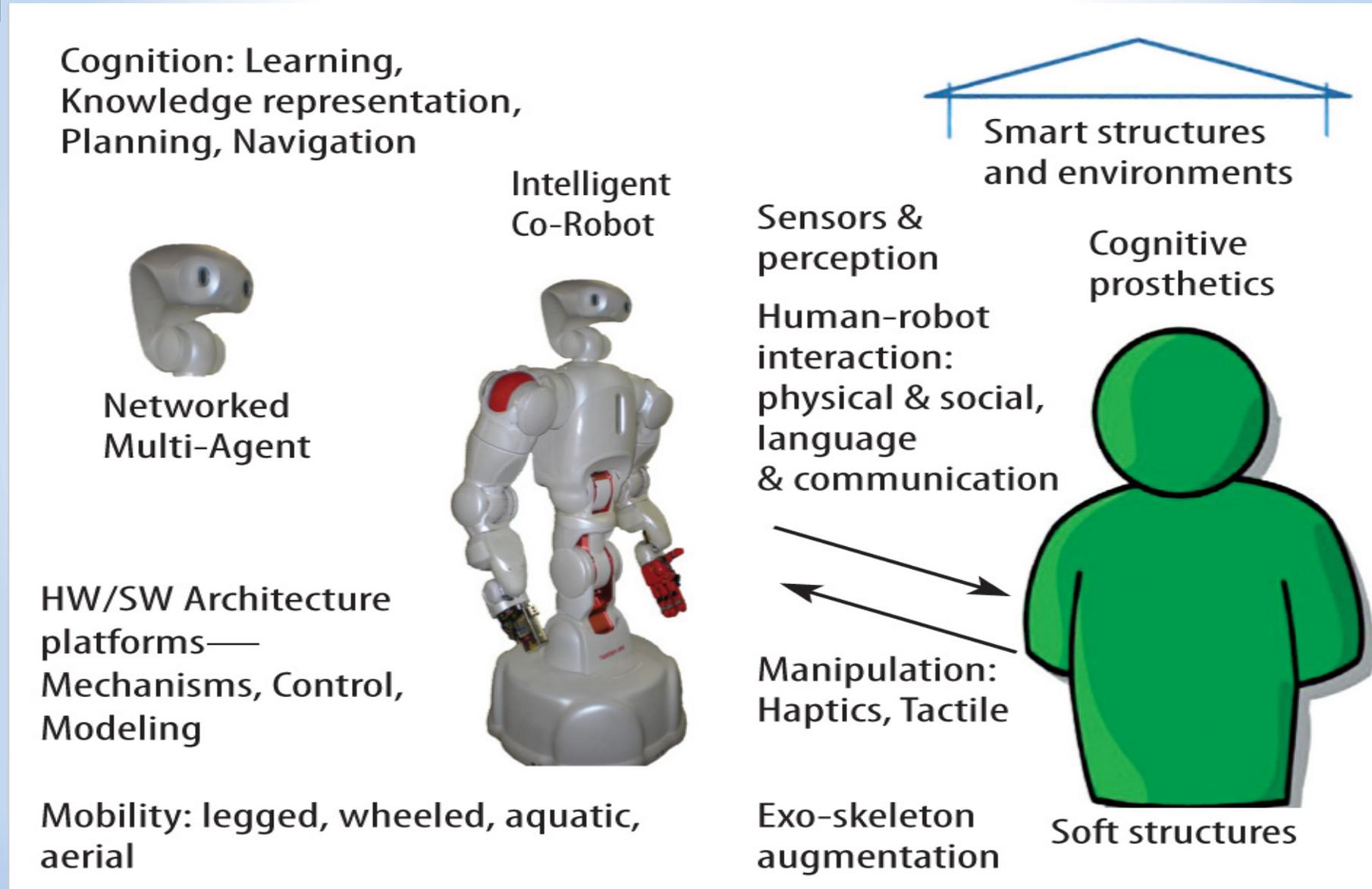
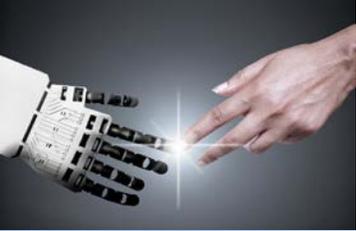
New system architectures



4D Analysis

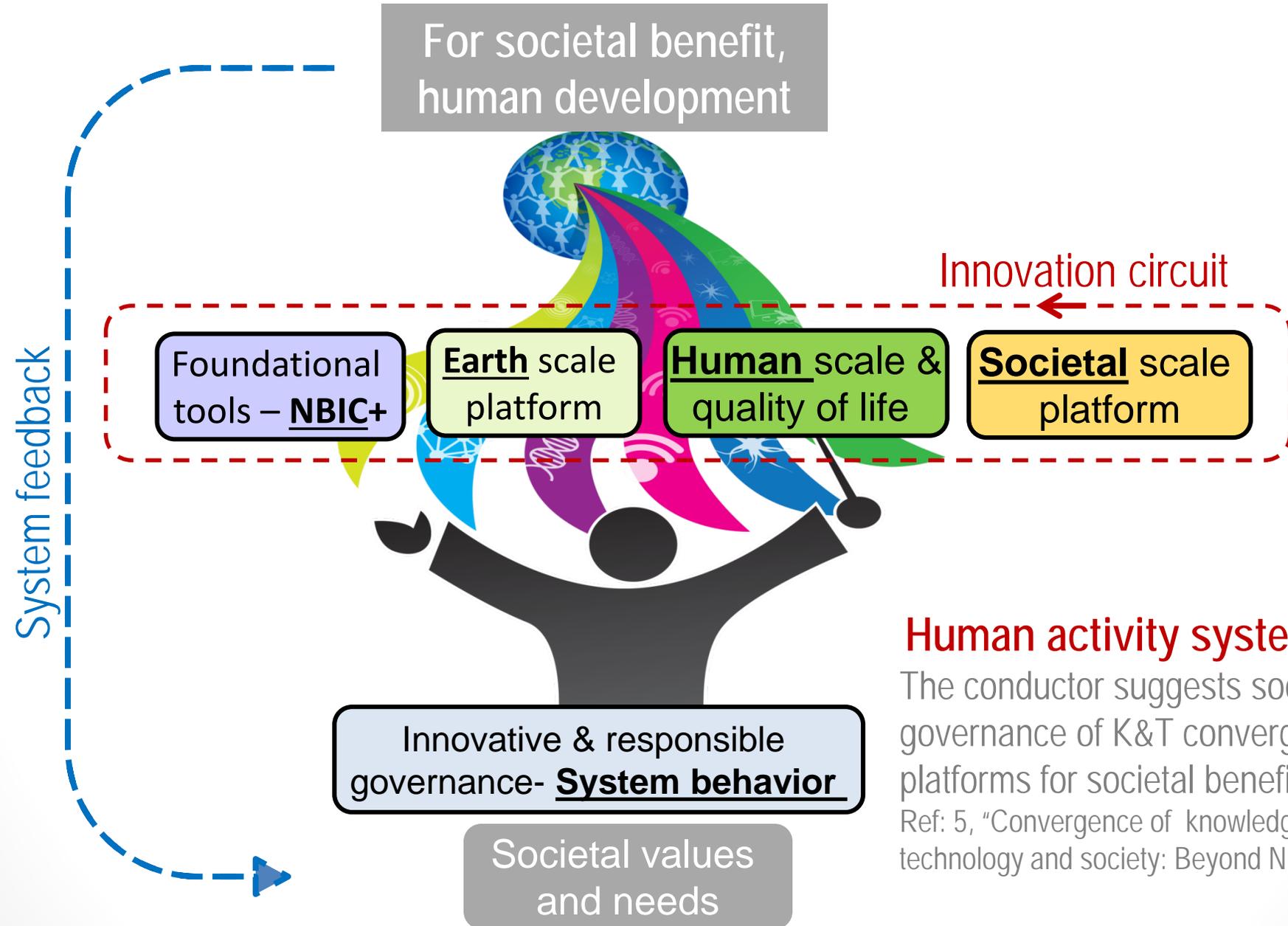
New concepts Computation

Human / co-robot interaction (National Robotics Initiative)





III. Convergence of Knowledge, Technology and Society



Human activity system

The conductor suggests societal governance of K&T converging platforms for societal benefit.

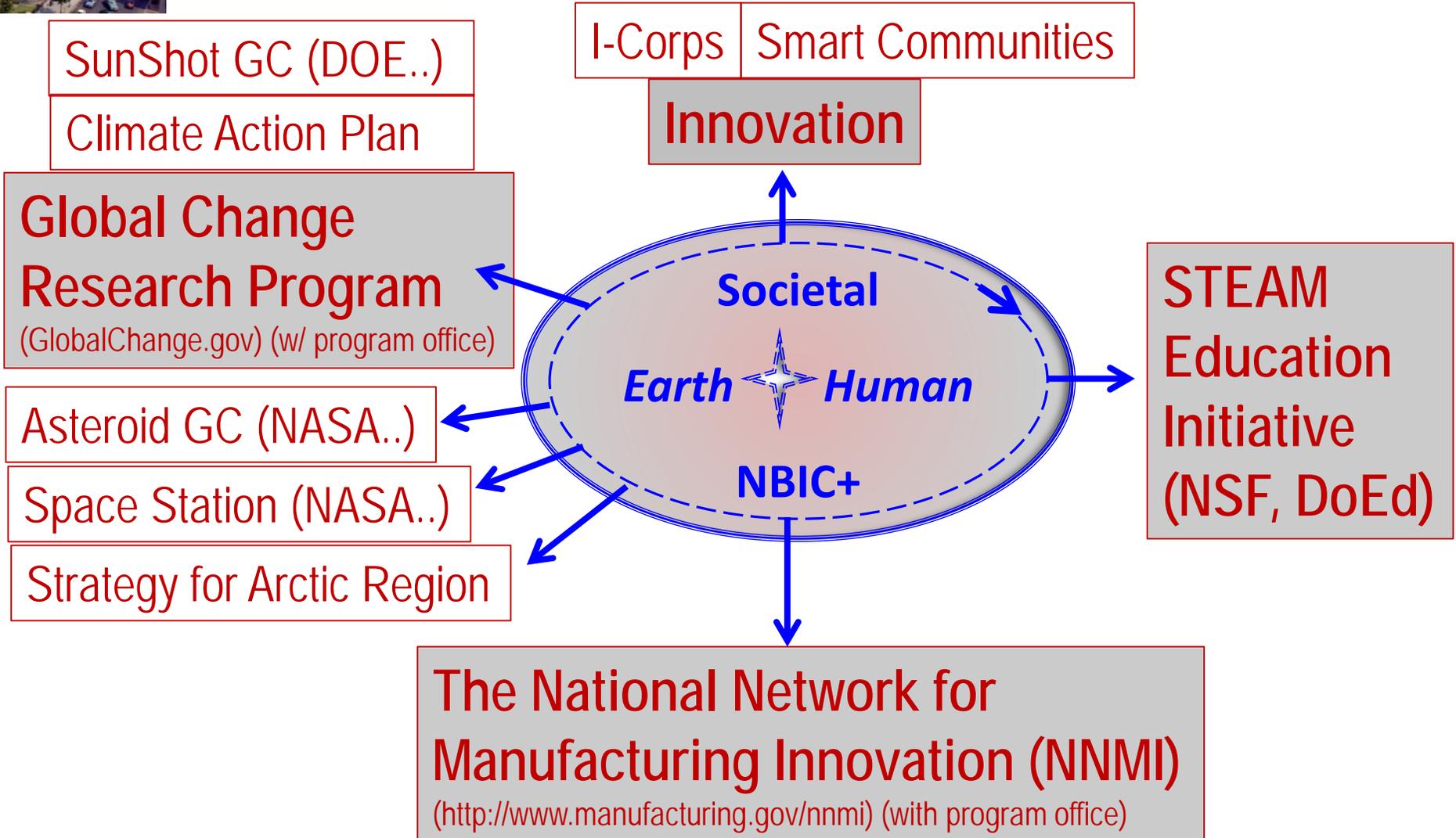
Ref: 5, "Convergence of knowledge, technology and society: Beyond NBIC"



Convergence of Knowledge and Technology (CKTS) leads to *U.S. global society-oriented initiatives*



OSTP



See Ref 9: "Principles and methods that facilitate convergence", Handbook of S&T Convergence, 2015

The National Network for Manufacturing Innovation (NNMI)

- 7 year plans -

Experiment in *ecosystem establishment* in “valley of death”

All the institutes will deal with nanotechnology to some extent

Current list - **10 institutes** (<http://manufacturing.gov/>):

- National Additive Manufacturing Innovation Institute (DoD/DOE) FY12
- Digital Manufacturing and Design Innovation (DoD) FY14
- Lightweight and Modern Metals Manufacturing (DoD) FY14
- Next Generation Power Electronics Manufacturing (DOE) FY14
- Clean Energy Manufacturing Innovation Institute for Composites Materials and Structures (DOE) FY15
- Photonics (DoD) FY15
- Hybrid Flexible Electronics (DoD) FY15
- Revolutionary Fibers and Textiles (DoD) FY16
- Two open competition centers (NIST) FY16-17

National Network of Manufacturing Institutes



Credit: B. Young/NIST

- Network of institutes focused on reducing cost and risk of commercializing transformative new technologies to address relevant manufacturing challenges on production-level scale
- President has asked Congress to authorize one-time \$1 billion investment—to be matched by private and other non-federal funds—to create initial network of up to 15 IMIs.



Other NSF specific initiative in 2016-

- Innovations at the Nexus of Food, Energy, and Water Systems
- Risk and Resilience
- Clean Energy Technology
- Cyber-Enabled Materials, Manufacturing, and Smart Systems
- Advanced Manufacturing
- Smart and Connected Communities
- Understanding the Brain, as a part of BRAIN Initiative
- Broadening Participation

NSF *INCLUDES*: Inclusion across the Nation of Communities of Learners that have been Underrepresented for Diversity in Engineering and Science
- Innovation Corps (I-Corps)



Critical Resilient Interdependent Infrastructure Systems and Processes (CRISP)

- Improves the resilience, interoperation, performance, and readiness of critical infrastructure
 - Advances knowledge of risk assessment and predictability
 - Supports novel tools, technologies, and engineered systems solutions for increased resilience
- CRISP initiative at NSF (ENG, CISE, and SBE)
 - Enhances understanding and design of interdependent critical infrastructure systems and processes that provide essential goods and services, both under normal conditions and despite disruptions and failures from any cause



Convergence-Divergence process (upstream): "Germination"

Germination of Research Ideas for Large Opportunities and Critical Societal Needs

- To design learning frameworks, platforms, and/or environments to enable participants to conceive research ideas and questions with potentially transformative outcomes
- NSF 16-028 Dear Colleague Letter for proposals
- Proposers were asked to focus on the development of key skills and mindsets that will increase the capacity of participants to Identify big opportunities, Think creatively, Explore novel research formulations, Take intellectual risk
Assess (a) Impact on participants (b) potential for scalability and adaptability



Convergence-Divergence process (downstream): **Innovation Corps (I-Corps™)**

- Provides experiential entrepreneurial education to capitalize on NSF investments in basic research
- Supports I-Corps™ Teams, Sites, and Nodes to build, utilize, and sustain a national innovation ecosystem
- Plans approximately 230 new I-Corps™ Teams, up to 71 active Sites, and up to 9 active Nodes in FY 2017
- Scaling via partnerships and networks: Federal agencies, states, private sector; and National Innovation Network



Smart and Connected Communities

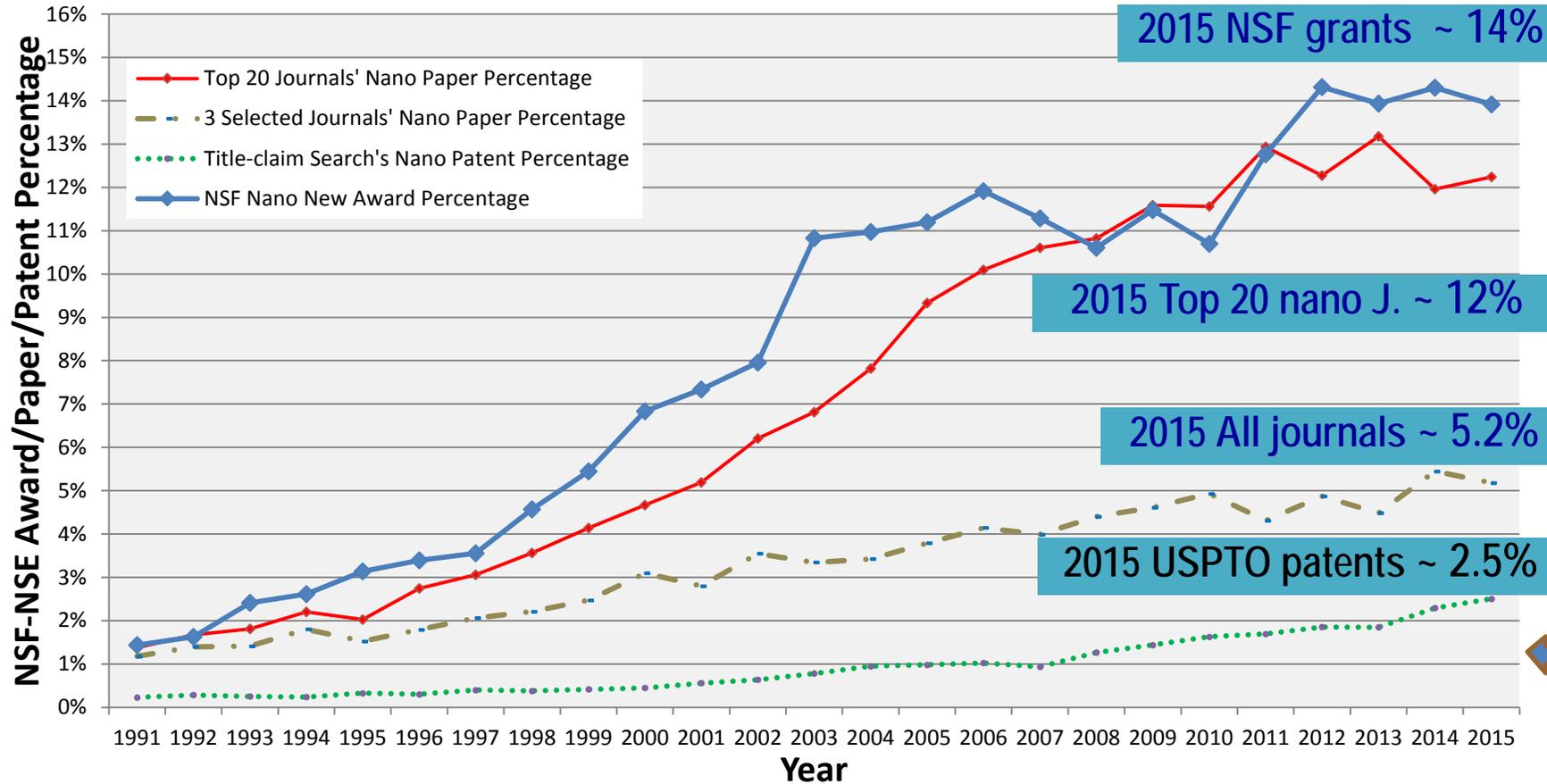
(OSTP and NSF)

- **Advances the integration of networked** computing systems, physical devices, data sources, and infrastructure to allow communities to surmount deeply interlocking physical, social, economic, and infrastructural challenges
- **FY 2016 DCL on Smart and Connected Communities**
 - ENG, CISE, EHR, GEO, and SBE
- **Dec. 2015 Workshop on Smart Cities**, Arlington, VA
- **Jan. 2016 Smart and Connected Communities: Planning Workshop**, Seattle, WA



Percentage rate of penetration of nanotechnology in NSF awards, WoS papers and USPTO patents (1991-2015)

Searched by keywords in the title/abstract/claims (update Encyclopedia Nanoscience, Roco, 2016)



Est. Market / US GDP: 2014 ~ 2% ; 2016 ~ 3% ; 2022 ~ 10% (if 25% market growth rate)

Global revenue from nano-enabled products by sector

(Lux Research, updated in January 2016) (US / World ~ 32%)

Sector <i>(all in US\$ Billion)</i>	2012 (survey)	2013 (survey)	2014 (survey)
Building materials	\$28.837	\$44.564	\$66.891
Materials & manufacturing	\$457.936	\$625.508	\$826.704
Electronics & IT	\$265.306	\$377.631	\$527.137
Healthcare & life sciences	\$74.742	\$103,350	\$139,597
Energy & Environment	\$25,668	\$38.478	\$55.737
Total (world)	\$853	\$1,190	\$1,616
<i>Annual Increase Rate (%)</i>		<i>40%</i>	<i>36%</i>

Nanotechnology-inspired Grand Challenges: Related publications

(4 reports with R&D recommendations for 2020)

1. *"The new world of discovery, invention, and innovation: convergence of knowledge, technology and society"* (Roco & Bainbridge, JNR 2013a, 15)
2. ***NANO1: "Nanotechnology research directions: Vision for the next decade"*** (Roco, Williams & Alivisatos, Springer, 316p, 2000), www.wtec.org/loyola/nano/IWGN.Research.Directions/
3. ***NANO2: "Nanotechnology research directions for societal needs in 2020"*** (Roco, Mirkin & Hersam, Springer, 690p, 2011a), www.wtec.org/nano2/
4. ***NBIC1: "Converging technologies for improving human performance: nano-bio-info-cognition"*** (Roco & Bainbridge, Springer, 468p, 2003), www.wtec.org/ConvergingTechnologies//1/NBIC_report.pdf
5. ***NBIC2: "Convergence of knowledge, technology and society: Beyond NBIC"*** (Roco, Bainbridge, Tonn & Whitesides; Springer, 604p, 2013b), www.wtec.org/NBIC2-Report/
6. *"Building Foundational Knowledge and Infrastructure for Nanotechnology: 2000-2030"*
Volume *"Nanotechnology: Delivering on the Promise"*, ACS, 2016, NY
7. *"Mapping nanotechnology innovation and knowledge: global and longitudinal patent and literature"* (Chen & Roco, Springer, 330p, 2009)
8. *"Principles and methods that facilitate convergence"*
(Roco, Springer Reference, Handbook of Science and Technology Convergence, 2015)
9. *"Handbook of Science and Technology Convergence"* (Springer, 700p, 2015)