



IMAG



4th Supercomputing Symposium
International Symposium for Next-Generation Integrated Simulation of Living Matter
(ISLiM), Tokyo, Japan
December 3, 2012

Grace C.Y. Peng, Ph.D.
National Institutes of Health (NIH)

WHAT CAN MULTISCALE MODELS DO FOR PRECISION MEDICINE?



The NIH

The NIH is an agency within the Department of Health and Human Services within the executive branch of the US government.

Its mission is science in pursuit of **fundamental knowledge** about the nature and behavior of living systems and the **application of that knowledge** to extend healthy life and reduce the burdens of illness and disability.



The NIH is the primary federal agency for conducting and supporting medical research in the US.



National Human
Genome Research
Institute



Clinical Center



NIAMS

National Institute of Arthritis and
Musculoskeletal and Skin Diseases



National Institute of
Biomedical Imaging
and Bioengineering



NATIONAL CENTER FOR COMPLEMENTARY
AND ALTERNATIVE MEDICINE



NATIONAL INSTITUTE ON AGING
National Institutes of Health



National Center for
Research Resources



National Institute of Diabetes and
Digestive and Kidney Diseases



National Institute of Dental
and Craniofacial Research



National Eye
Institute
NATIONAL INSTITUTES OF HEALTH



NIEHS
National Institute of
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NIDA
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FOGARTY
International Center



NATIONAL
CANCER
INSTITUTE



National Heart
Lung and Blood Institute



National Institute
of Allergy and
Infectious Diseases



NIAAA
National Institute on Alcohol
Abuse and Alcoholism



NIDCD
National Institute of
Deafness and
Communications Disorders

27 Separate Institutes &
Centers (IC) each with
different:

- missions & priorities
- budgets
- ways of deciding which grants to fund

NATIONAL INSTITUTES
OF HEALTH

The **NIBIB** Mission

Improving human health by leading the **development and accelerating the application of biomedical technologies.**

The Institute is committed to **integrating the physical and engineering sciences with the life sciences** to advance basic research and medical care.



The NIBIB **Vision**

**To profoundly change health care
by pushing the frontiers of
technology to make the possible a
reality.**



Non-Hypothesis Driven Research

There are two kinds of scientific revolutions, those driven by new tools and those driven by new concepts... The effect of a concept-driven revolution is to explain old things in new ways. The effect of a tool-driven revolution is to discover new things that have to be explained.

-Freeman Dyson, 1997



NIBIB supports

- Design- and needs-driven research, as well as hypothesis-driven
- Focus on enabling technologies with broad applications to multiple diseases or biological processes
- Multi-disciplinary and collaborative research
- Inter-agency and inter-institute activities

NIBIB Program Areas

- Biomaterials
- Biomedical Informatics
- Drug & Gene Delivery Systems and Devices
- **Mathematical Modeling, Simulation and Analysis**
- Medical Devices and Implant Science
- Micro-Biomechanics
- Micro- and Nano Systems; Platform Technologies
- Nanotechnology
- Rehabilitation Engineering (Robotics)
- Sensors
- Structural Biology
- Surgical Tools, Techniques and Systems
- Telehealth
- Tissue Engineering
- Image-Guided Interventions
- Image Processing, Visual Perception and Displays
- Magnetic, Biomagnetic and Bioelectric Devices
- Magnetic Resonance Imaging & Spectroscopy
- Molecular Imaging
- Nuclear Medicine
- Optical Imaging & Spectroscopy
- Ultrasound: Diagnostic and Interventional
- X ray, Electron, and Ion Beam



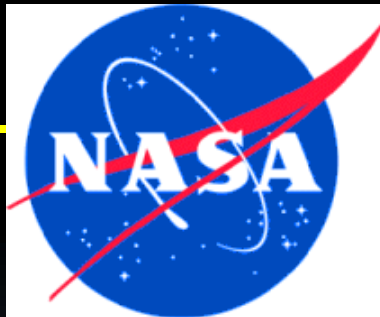
Modeling is a tool
or platform that is
severely underused
to study complex
biological systems



IMAG



Interagency Modeling and Analysis Group

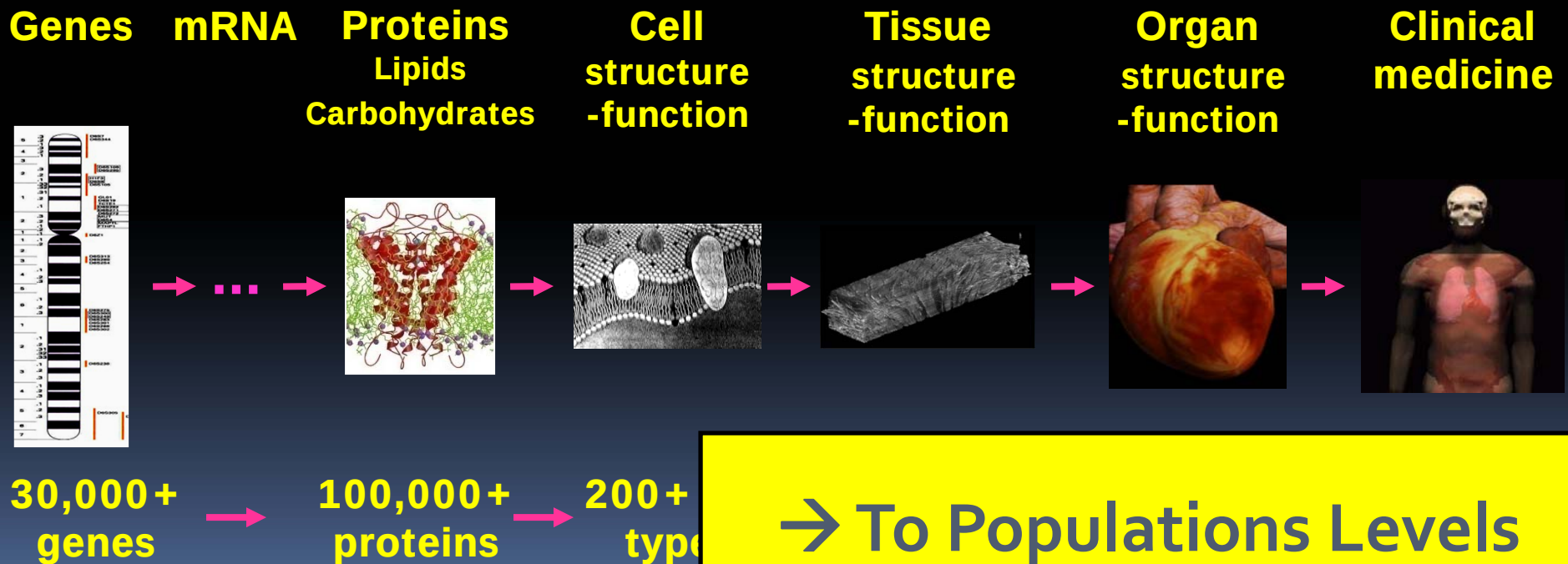


The Intelligence Advanced Research Projects Activity (IARPA)

Multiscale Modeling

Multi-scale modeling deals with spanning scales from molecular to population and is expected to largely impact the understanding of biological processes and also further the predictive capability in biological, biomedical and environmental systems. Multi-scale modeling encompasses concepts of space, time and state space.

Biological Scales



IMAG Activities

- 2003 - Created
- 2004 - Interagency Solicitation for Multiscale Modeling in Biomedical, Biological and Behavioral Systems (NIH, NSF, NASA, DOE)
- 2006 – Formation of the MSM Consortium
- 2007 - Predictive Multiscale Models of the Physiome in Health and Disease (R01)
- 2009 – IMAG Futures Meeting
- 2011 - Predictive Multiscale Models for Biomedical, Biological, Behavioral, Environmental and Clinical Systems (Interagency U01) (NIH, NSF, DOE, FDA)

Interagency Modeling and Analysis Group (IMAG)Wiki (Google: IMAG Wiki)



Search

Go

Search

Navigation

Main Page
Events
Webinars
Working Groups
Modeling
Resources
Discussion Forum
VPH Network
Population Modeling
Recent changes

Support

Getting Started
Wiki Editing Help
Wiki Text Formatting
Adding Links to Wiki
Creating a New Wiki Page
Uploading Documents and Images

Toolbox

What links here

WELCOME TO THE IMAG WIKI

This wiki contains information relevant to the [IMAG](#) (Interagency Modeling and Analysis Group) and the [MSM](#) (Multi-scale Modeling Consortium).

Questions about IMAG and the MSM Consortium can be directed to
Dr. Grace Peng: penggr@mail.nih.gov

- [MSM Consortium FAQ](#)
- [MSM Participants](#)
- [IMAG Participants](#)
- [IMAG Agencies](#)
- [About the Wiki](#)

Announcements

October 22-23 at NIH Main Campus 2012 MSM CONSORTIUM MEETING

feedback and suggestions for next year's meeting! 2012 MSM Planning Feedback

- Editorial published on the 2009 IMAG Futures Meeting
 - [IEEE Transactions on Biomedical Engineering](#)
 - Editorial: **What Biomedical Engineers can do to Impact Multiscale Modeling** (TBME Letters Special Issue on Multiscale Modeling and Analysis in computational Biology and Medicine: Part-2)

Webinars

- **Wed Nov 14 at 12:30pm ET: Multiscale Systems Biology Presentation**
Modeling cardiac function and dysfunction -Natalia Trayan
Adobe Connect: <https://webmeeting.nih.gov/r61727550/>
in: 1-866-546-3377, passcode: 474962
- **Mon Nov 19 at 1:00pm ET: Awardee Linda Petzold**
Stochastic Simulation Service: Towards an Integrated Development Environment for Modeling and Simulation of Stochastic Biochemical Systems
Adobe Connect: <https://webmeeting.nih.gov/r94341812/>
in: 1-866-546-3377, passcode: 474962
- **Wed Nov 28 at 1:00pm ET: Awardee Xiaobo Zhou**
Modeling the Growth of the MIC Niche at the System Level
Adobe Connect: <https://webmeeting.nih.gov/r12932671/>
in: 1-866-546-3377, passcode: 474962

All Webinars

Funding Opportunities

Upcoming Meetings

Participation Welcome!

The MSM Consortium provides opportunities to:

- converse with program officers from 10 government agencies, [IMAG Participants](#), from the United States and Canada
- network with other MSM investigators, [MSM Participants and Projects](#)
- participate in [Working Group](#) discussions on the wiki
- participate in virtual scientific presentations by all [Working Groups](#) throughout the year
- participate in annual meetings of the MSM Consortium, [IMAG/MSM Events](#)
- learn about the latest modeling and MSM related activities from around the world, [Multiscale Modeling of the Physiome - Projects Around the World](#)
- access various [Resources for Modeling](#)

The logo for IMAG (Institute for Modeling and Analysis of the Genome) is displayed in the bottom right corner. It features the word "IMAG" in a large, bold, serif font. The letters are white with a blue outline and a subtle gradient, giving it a three-dimensional appearance. The background of the logo is a dark blue gradient.

2012 MSM Working Groups

- Multiscale Systems Biology Working Group
- Biomechanics Working Group
- Theoretical and Computational Methods
- Model Sharing Working Group
 - Automated Reconstruction of Models
 - VV&UQ
- Data Sharing Working Group
- Clinical and Translational Issues Working Group
- Computational Neuroscience Working Group
- Population Modeling Working Group
- High Performance Computing Working Group

[page](#)[discussion](#)[edit](#)[history](#)[move](#)[watch](#)

High Performance Computing Working Group

search

navigation

- [Main Page](#)
- [Events](#)
- [Webinars](#)
- [Working Groups](#)
- [Modeling](#)
- [Resources](#)
- [Discussion Forum](#)
- [VPH Network](#)
- [Population Modeling](#)
- [Recent changes](#)

support

- [Getting Started](#)
- [Wiki Editing Help](#)
- [Wiki Text Formatting](#)
- [Adding Links to Wiki](#)
- [Creating a New Wiki Page](#)
- [Uploading Documents and Images](#)

toolbox

- [What links here](#)

Contents [\[hide\]](#)

- 1 [High Performance Computing Working Group](#)
 - 1.1 [Goals and Objectives:](#)
 - 1.2 [Participation in Working Group:](#)
 - 1.3 [Upcoming Presentations](#)
 - 1.4 [Past Presentations](#)
 - 1.5 [Relevant Infrastructure:](#)
 - 1.6 [Challenges and Opportunities:](#)
 - 1.7 [References:](#)
 - 1.8 [List of Participants:](#)

High Performance Computing Working Group

Working Group leads: [Pratul Agarwal](#) , [Yufang Jin](#) 

Goals and Objectives:

The goal of this working group is to initiate discussion, foster collaboration and data sharing including (but not limited) to:

1. Computational resources including high performance computing.
2. Multi-scale modeling and simulations on emerging computer architectures (e.g. GPUs).
3. Computational algorithms, libraries, tool-kits and software.
4. Infrastructure and strategies to handle *big-data* problems.

Participation in Working Group:

Evolved from [Working Group 5](#).

Currently, feed-back is being sought from various members of the community regarding the need and availability of the computing re

Please send your responses by e-mail to the working group leads. Single word responses (yes/no) or responses to partial list a

Topic: Computing Hardware Resources

1. Some researchers already have access to what they need (computers, university clusters, storage space) but not everybody

Promoting Global Cooperation and Awareness

<http://www.imagwiki.org/mediawiki>



search

Go Search

navigation

- Main Page
- Events
- Webinars
- Working Groups
- Modeling
- Resources
- Discussion Forum
- VPH Network
- Population Modeling
- Recent changes

support

- Getting Started
- Wiki Editing Help
- Wiki Text Formatting
- Adding Links to Wiki
- Creating a New Wiki Page
- Uploading Documents and Images

toolbox

Japan

Notice of Availability of Administrative Supplements for the U.S.-JAPAN Brain Research Coop

This Notice supports 1) visits of U.S. scientists to conduct collaborative research and/or to acquire advanced research skills in Japanese information and to foster collaborations.

Receipt date: September 15, 2010-2012

- [More Information](#)

Next-Generation Integrated Simulation of Living Matter

http://www.csrp.riken.jp/index_e.html

- Newsletters
- Biosupercomputing Symposium Pages

University of Tokyo Heart Simulator

<http://www.sml.k.u-tokyo.ac.jp/index.html>

Leading Project for Biosimulation

<http://www.lp-biosimulation.com/english/index.shtml>

MEI center in silico medicine

<http://www.mei.osaka-u.ac.jp/gCOE/english/index.html>

National Institute for Physiological Sciences

<http://www.nips.ac.jp/eng/>

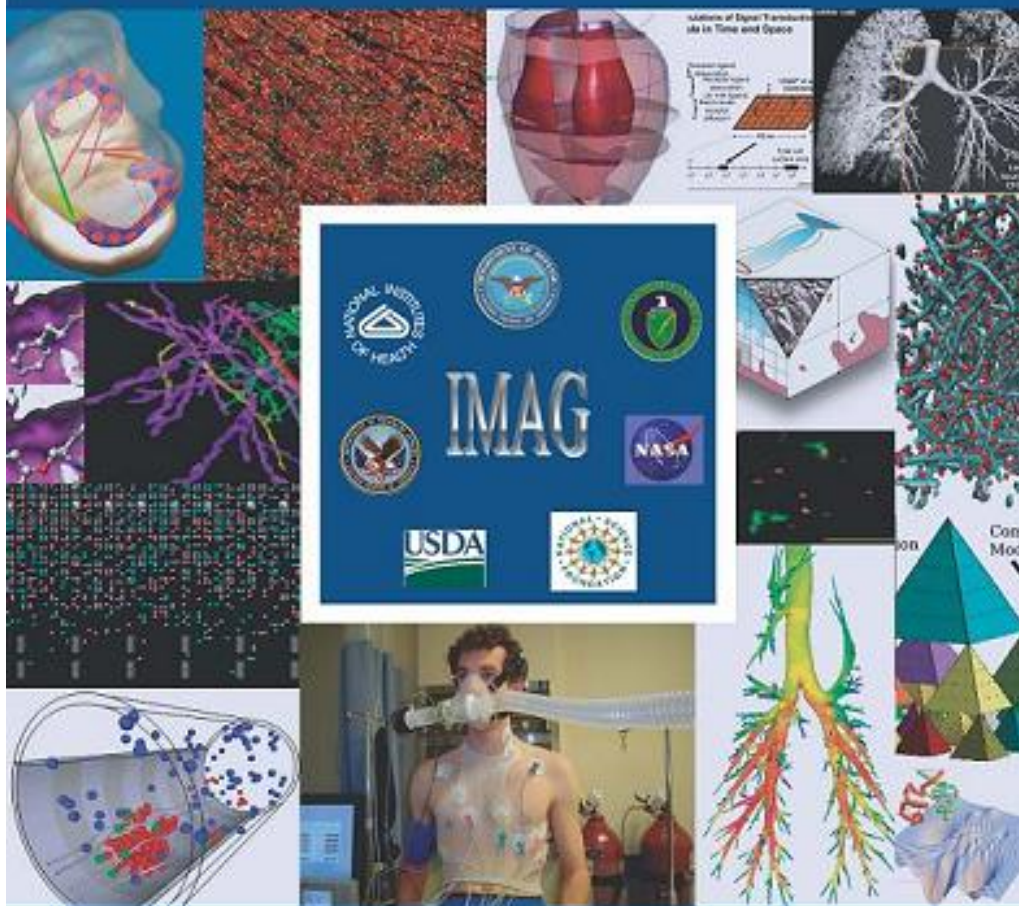
Unique Resources and Expertise

Japan model sharing survey - Summary Report of 2008 SIAM Forward Looking Session

Interagency Modeling and Analysis Group (IMAG)

3rd Annual Multiscale Modeling (MSM) Consortium Meeting

August 4-7, 2008 • Montreal, Canada



FIFTH MEETING

MULTISCALE MODELING CONSORTIUM

IMAG

INTERAGENCY MODELING & ANALYSIS GROUP



A JOINT SYMPOSIUM WITH THE
NHLBI SYSTEMS
BIOLOGY GRANTEES

OCTOBER 5-6, 2011
ROCKVILLE, MD



2012 MSM Consortium Meeting

October 22-23, 2012

Theme Focus: MSM for Precision Healthcare

- Panel 1 -- Data-driven models, physiological models and structural models – can they be tailored to individuals for precision healthcare?
- Panel 2 -- Can computational biology facilitate precision healthcare?
- Panel 3 -- How can we utilize clinical data to inspire MSM research for precision healthcare?
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The NEW ENGLAND JOURNAL of MEDICINE

Journal of Mental Health
treatment of mental illness through research

Search

Funding

News Room

Educational Resources

HOME

ARTICLES & MULTIMEDIA

ISSUES

SPECIALTIES & TOPICS

FOR AUTHORS

CME

Medicine



Perspective

Preparing for Precision Medicine

Reza Mirnezami, M.R.C.S., Jeremy Nicholson, Ph.D., and Ara Darzi, M.D.

N Engl J Med 2012; 366:489-491 | February 9, 2012 | DOI: 10.1056/NEJMp1114866

new report titled

Biomedical Research and a New Taxonomy of

diagnosis in medicine, based on a multi-level

Toward analysis of disease, from genomic risk to the "exposome" — essentially a characterization of both external and internal exposures that can affect how a person is predisposed to disease at various life stages

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The Lancet, Volume 378, Issue 9804, Page 1678, 12 November 2011

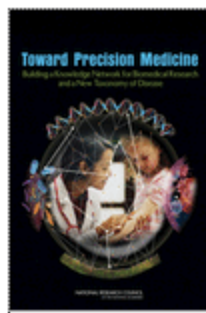
doi:10.1016/S0140-6736(11)61725-X [Cite or Link Using DOI](#)

< [Previous Article](#) | [Next Article](#) >

Moving toward precision medicine

[The Lancet](#)

The century-old International Classification of Diseases (ICD) is well known to epidemiologists and public health specialists, but little used in other areas of clinical research. New insights into human disease are emerging from basic research, and this explosion of information has the potential to revolutionise disease diagnosis, therapeutics, and clinical decision-making. Is a new taxonomy of human disease based on molecular and cell biology needed?



[Read/Purchase](#)

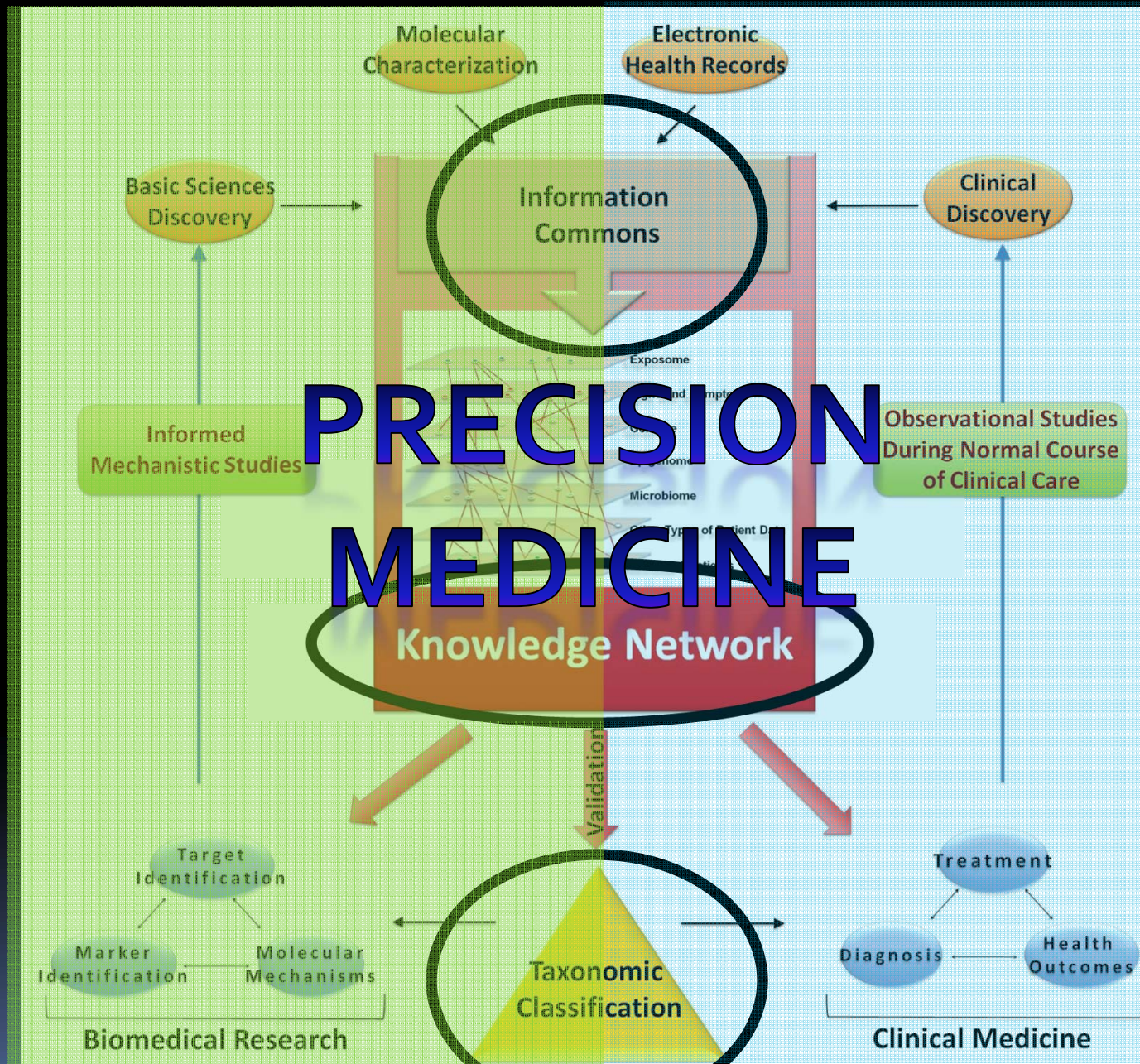
Understanding Diseases



From Bottom-Up

From Top-Down





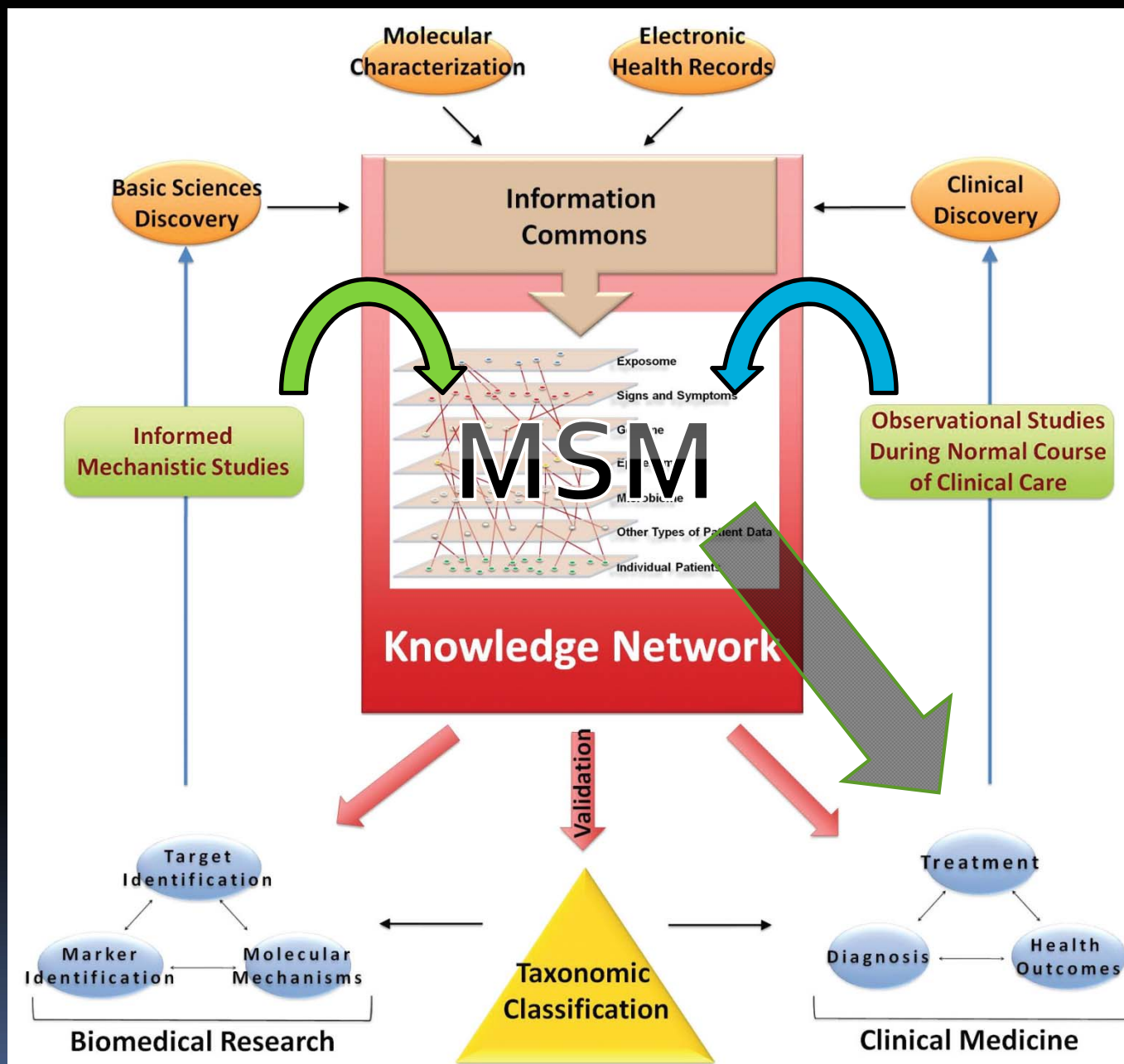
TOWARD PRECISION MEDICINE, NAS 2011

2012 MSM Consortium Meeting

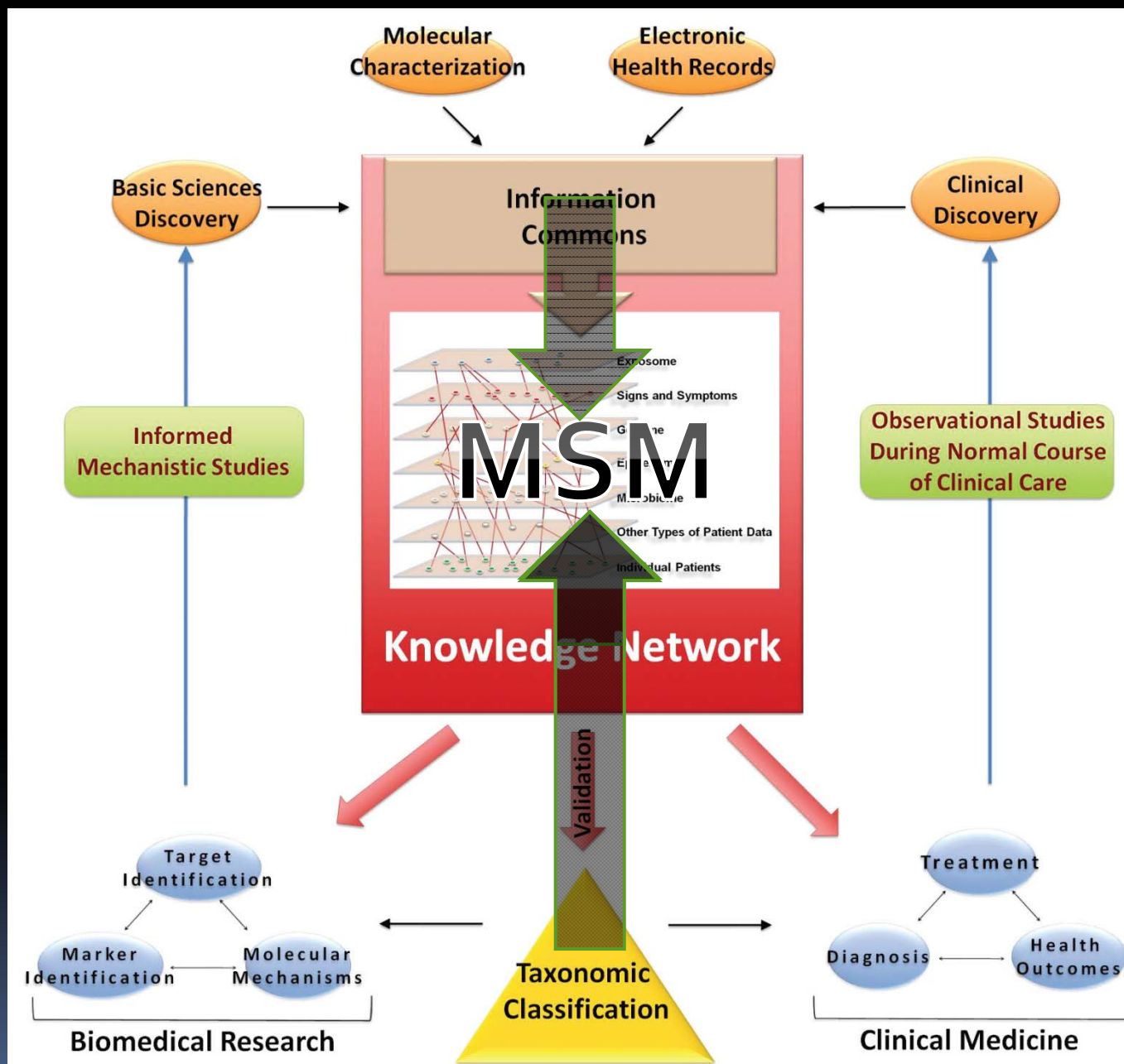
October 22-23, 2012

Theme Focus: MSM for Precision Healthcare

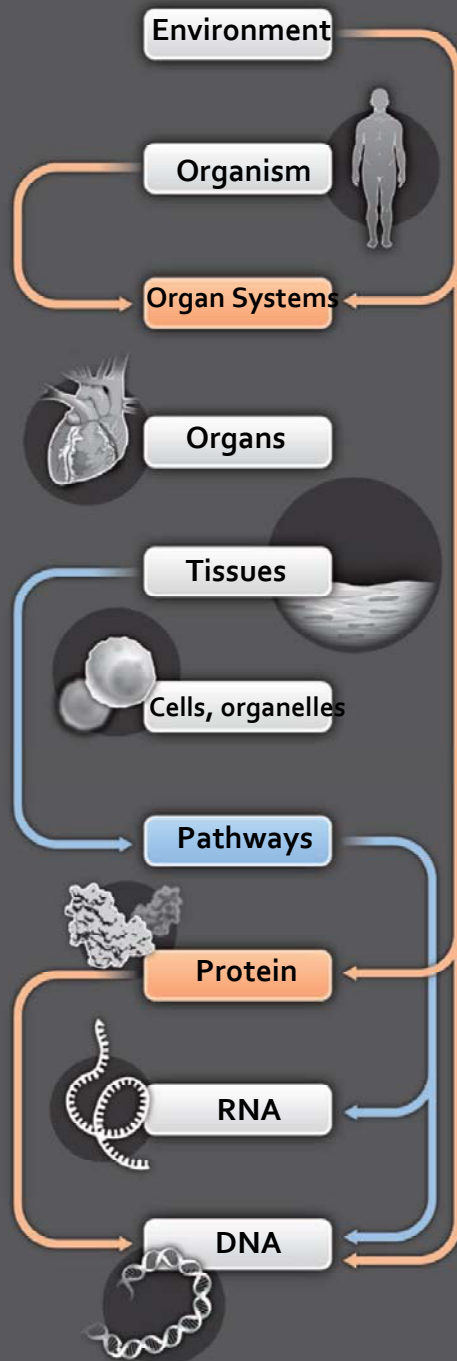
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TOWARD PRECISION MEDICINE, NAS 2011



TOWARD PRECISION MEDICINE, NAS 2011



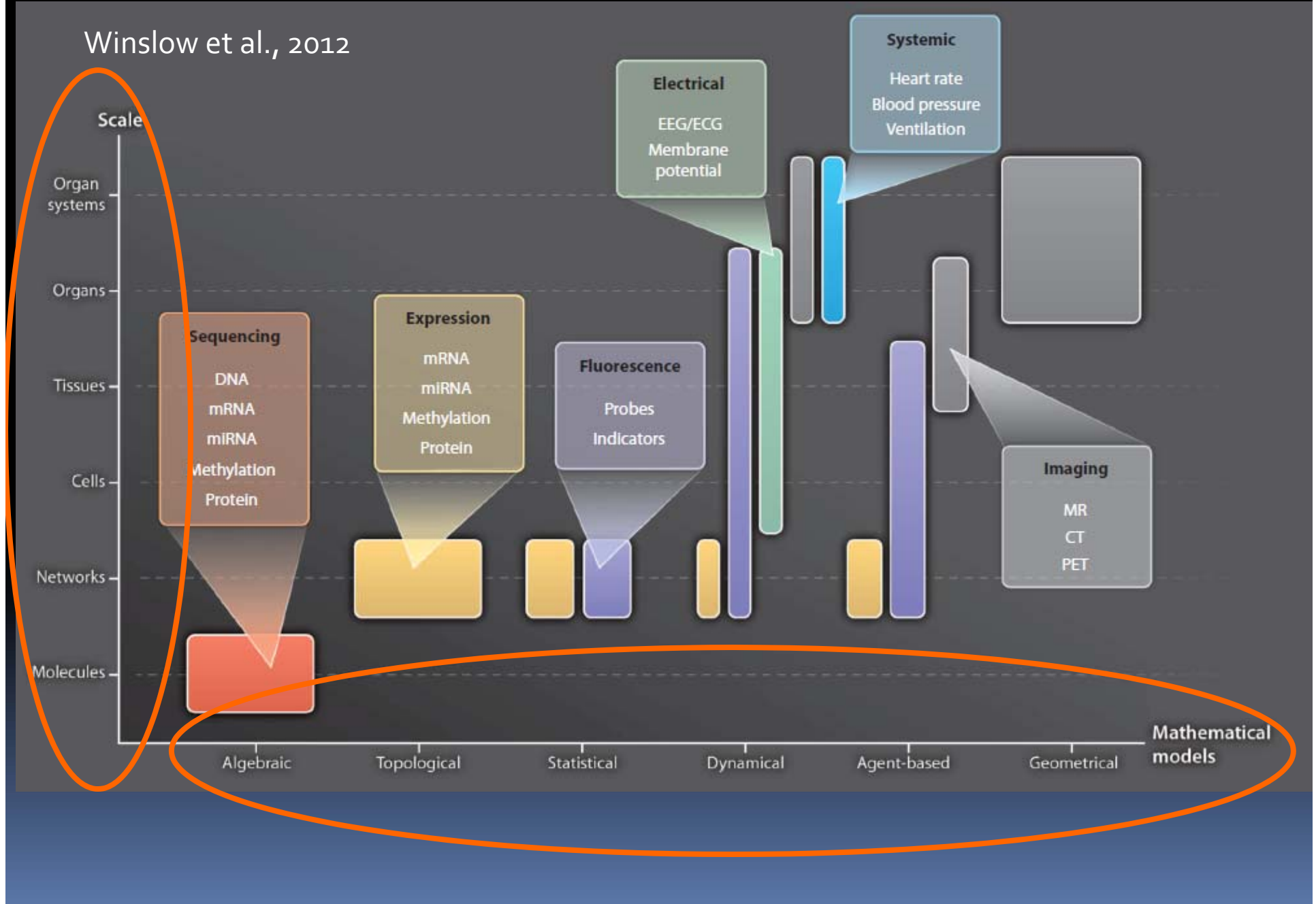
Physiological Function

Distributed across multiple biological scales

"...understanding physiological systems in health and disease can only be achieved through quantitative modeling and cannot be understood using "mental models.""

Winslow et al., 2012

Winslow et al., 2012



2012 MSM Consortium Meeting

October 22-23, 2012

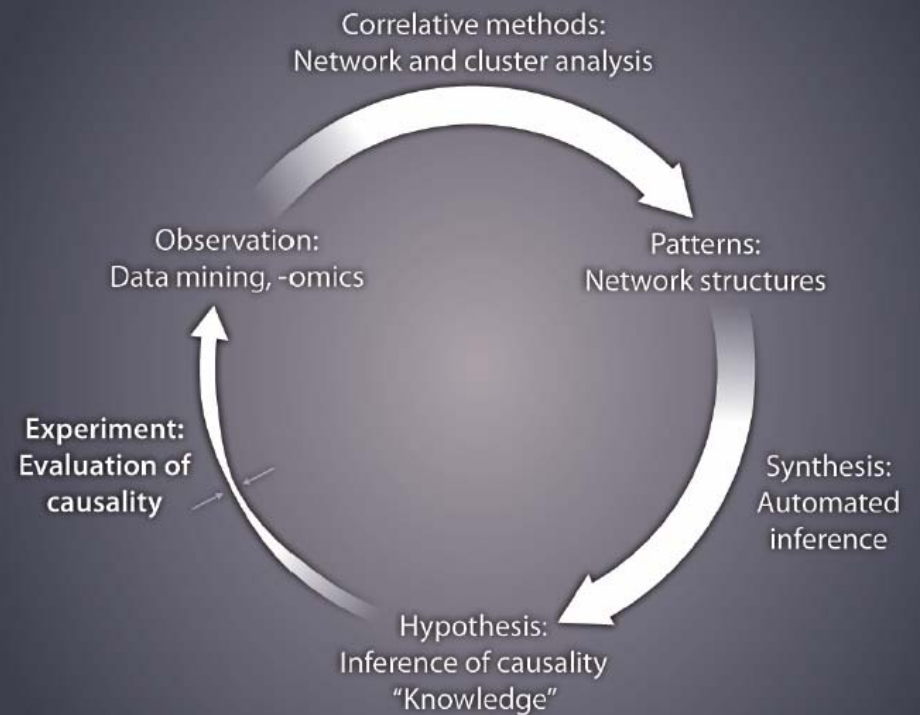
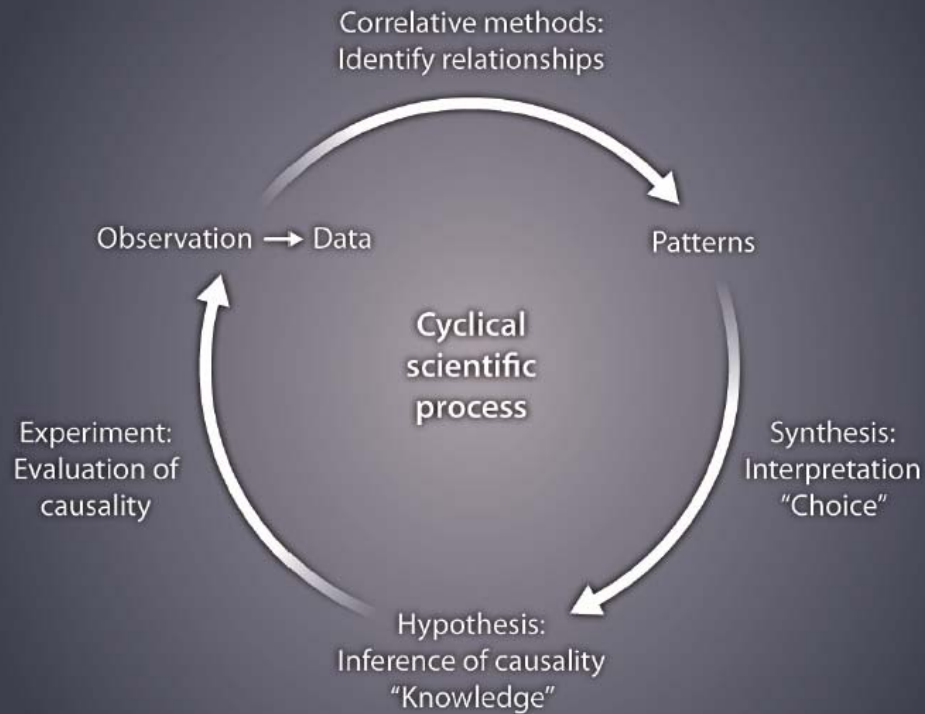
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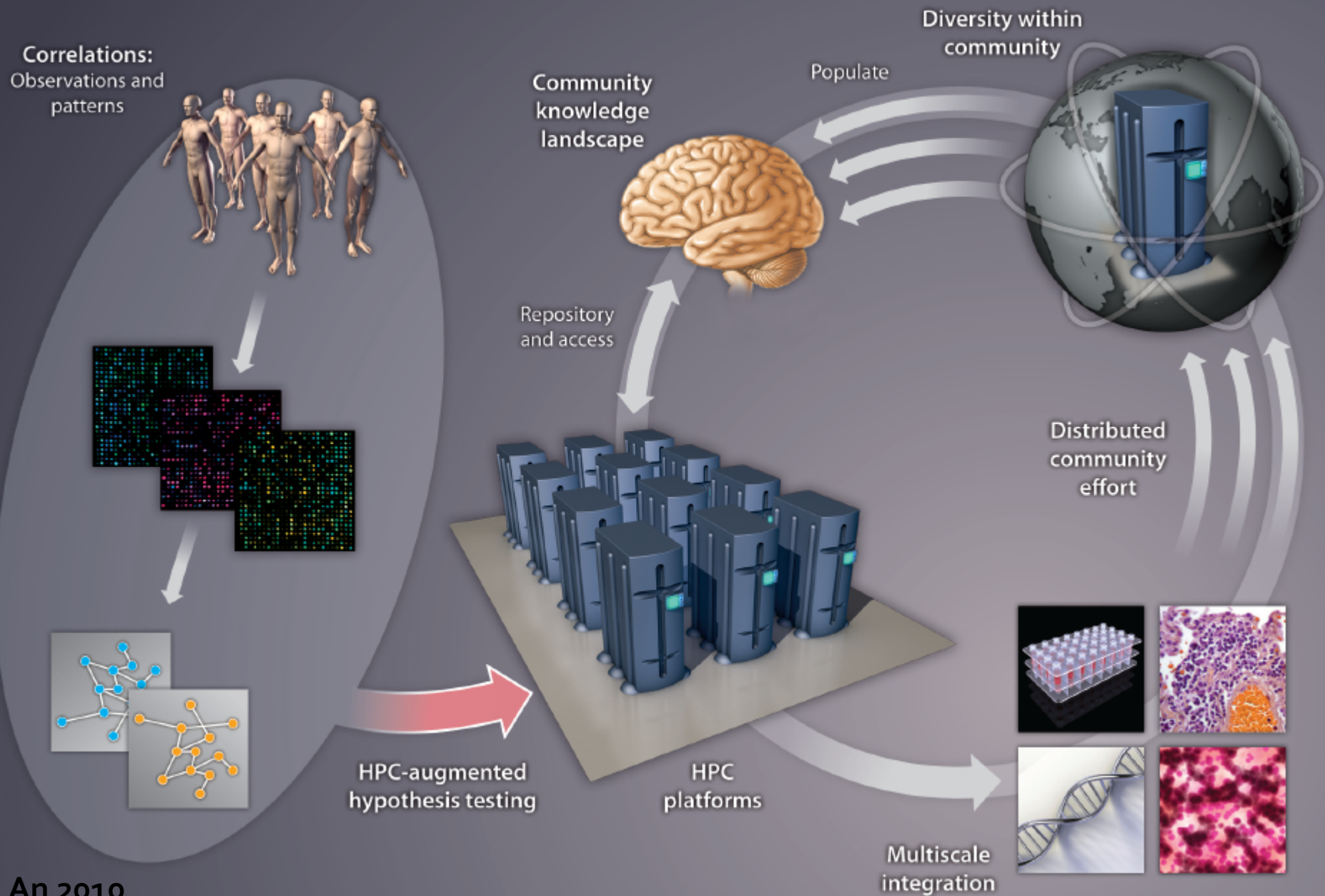
An 2010

Present

Past



The Future with High Performance Computing





General Information

print 

biology

Quantitative and Systems Pharmacology in the Post-genomic Era: New Approaches to Discovering Drugs and Understanding Therapeutic Mechanisms

An NIH White Paper by the QSP Workshop Group – October, 2011

Peter K. Sorger (co-chair), Sandra R.B. Allerheiligen (co-chair)

Darrell R. Abernethy, Russ B. Altman, Kim L. R. Brouwer, Andrea Califano, David Z. D'Argenio, Ravi Iyengar, William J. Jusko, Richard Lalonde, Douglas A. Lauffenburger, Brian Shoichet, James L. Stevens, Shankar Subramaniam, Piet Van der Graaf and Paolo Vicini

Quantitative Systems Pharmacology

Recommendations

- Move beyond characterizing drug/target interactions to a holistic quantitative understanding of drug action across many levels
 - from drug-receptor interactions to drug response in humans
- Require the participation of scientists from academia and industry who work in diverse areas
 - including traditional pharmacology, clinical pharmacology, pharmacodynamics/pharmacokinetic modeling, systems biology, chemistry, bioinformatics, multiscale modeling and computer science
- Training new and established investigators also will be a critical element

Develop **multi-scale computational models** of pharmacological mechanism that span the divide between cell-level biochemical models and organism-level PK/PD models

- **Develop better quantitative models of pharmacological mechanism at all scales**
 - starting with single targets and drugs and scaling to vertically and horizontally integrated multi-scale models
- **Advance the state of the art in modeling mammalian signaling networks and their perturbation by drugs**
- **Improve dissemination of these models with transparent and effective means to explore QSP models of different types**
 - web-based modeling environments
 - cloud-based computing

2012 MSM Consortium Meeting

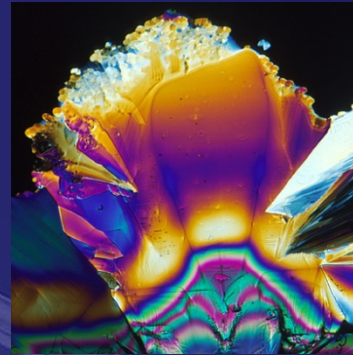
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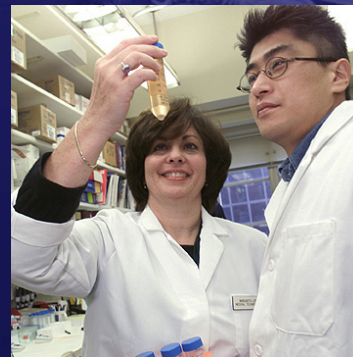
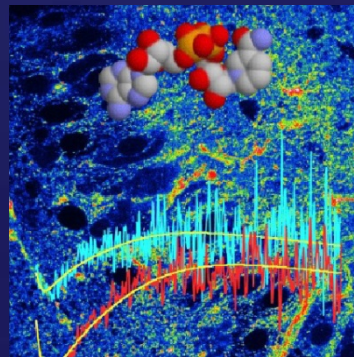
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Bridging Models with Clinical Data

- Direct connections between clinical findings & physiological models
- Include “subjective” clinical feedback in models
- Utilize models to control parameters used for clinical treatment
- Link information from individuals to look at population distribution of responses
- Definition of “clinical data” may change
- Clinician acceptance is dependent on model validation – huge hurdle
- Need to collaborate with clinicians
- Make models easily useable by clinicians
- Invest in data repositories for clinical model development



NIH *Transforming medicine through discovery*



IMAG plans for 2013

- Create a clinical model index on the IMAG wiki
- Categorize models by disease & conditions
- Bring in clinical societies, groups into the discussion
- Incorporate activities into 2013 MSM Consortium meeting

2012 MSM Consortium Meeting

October 22-23, 2012

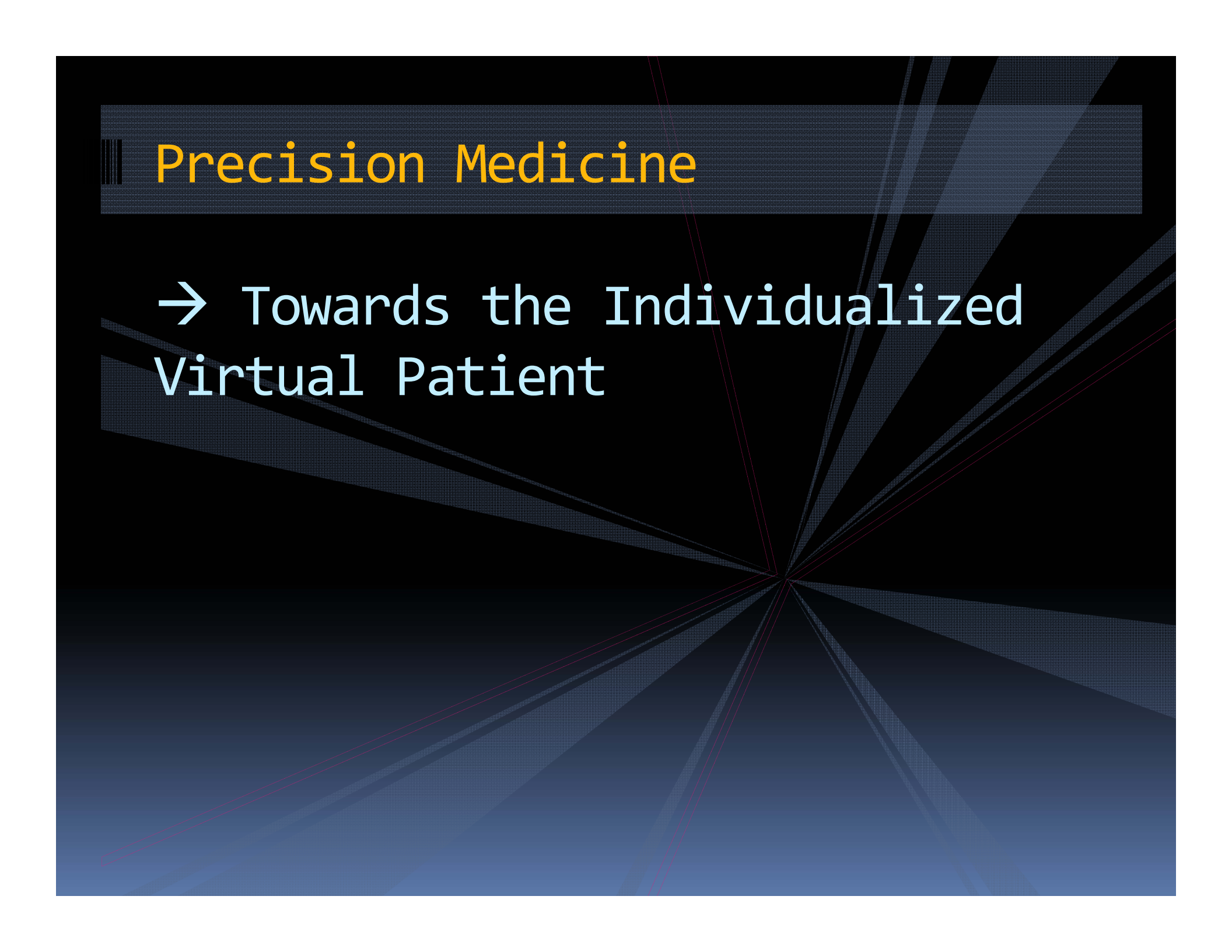
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“ALL MODELS ARE WRONG BUT
SOME ARE USEFUL”

“...the practical question is how wrong do they
have to be to not be useful.”

George Box, 1979



Precision Medicine

→ Towards the Individualized
Virtual Patient

Verification

The process of determining that a computational model accurately represents the underlying mathematical model and its solution.

“solving the equations right”

Validation

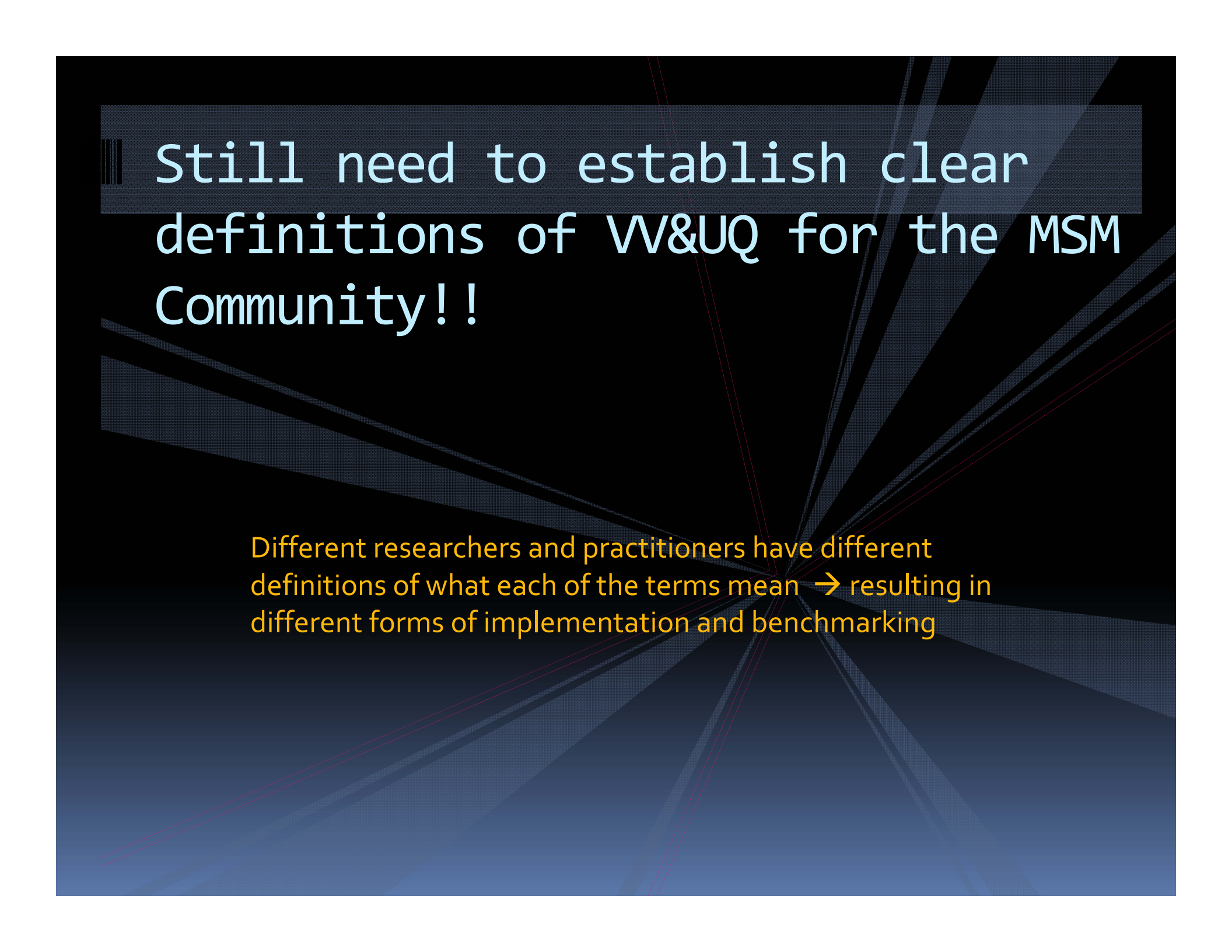
The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

“solving the right equations”

Uncertainty Quantification

The process of quantifying all sources of error and uncertainty in a model-based prediction of the quantities of interest.

“probability that the model prediction is right”



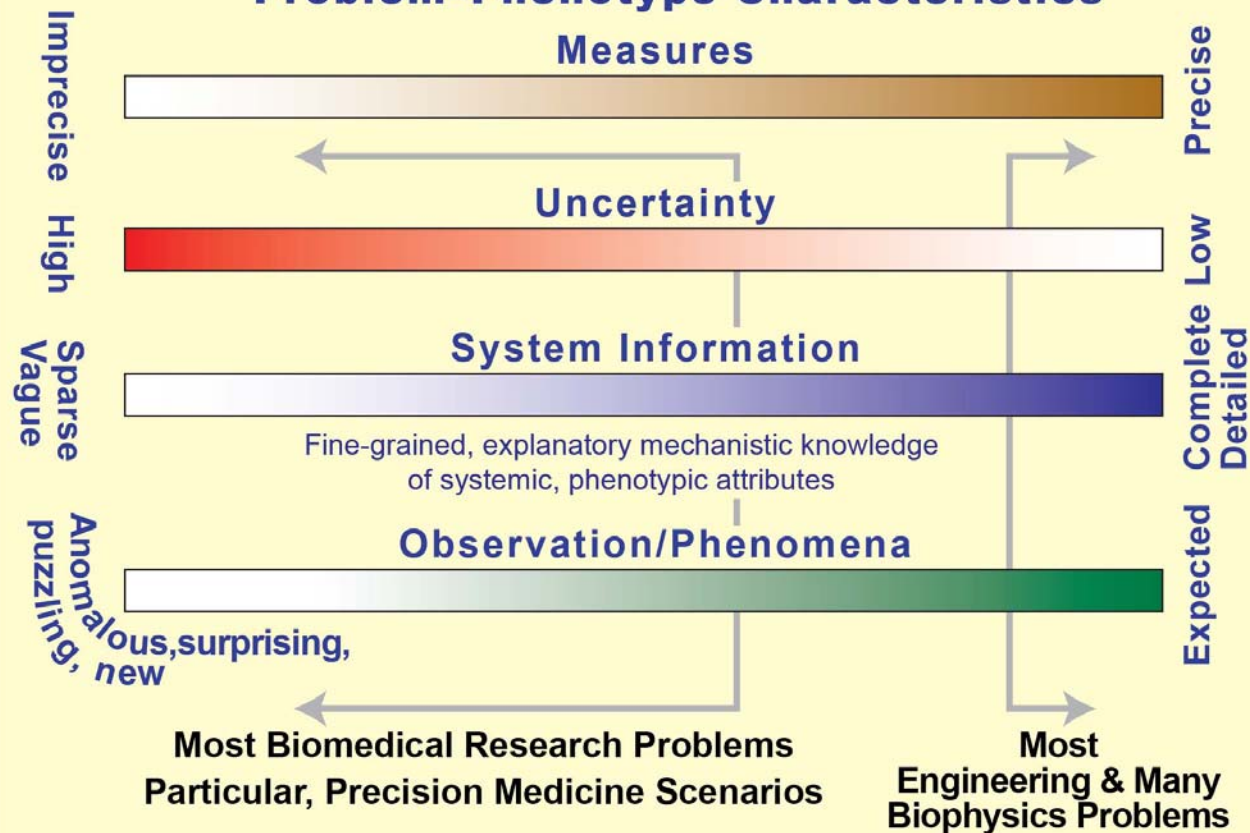
Still need to establish clear definitions of VV&UQ for the MSM Community!!

Different researchers and practitioners have different definitions of what each of the terms mean → resulting in different forms of implementation and benchmarking

Conditions More Supportive of:

← Abductive reasoning	Inductive/deductive reasoning →
← Synthetic mechanistic MSM	Inductive/deductive mechanistic MSM →
← OO, AB, Actor	Continuous mathematics →
← Relational grounding	Absolute grounding →
← Discovery/exploration	Precise predictions →

Problem-Phenotype Characteristics Measures



Key Considerations for VV&UQ

- **Consider the conceptual models**
 - Are there several? Are they stable or evolving? To what extent have they survived rounds of experimental challenge (wet-lab, clinical, translational, & in silico)?
- **Consider the wet-lab/clinical data on which conceptual models were based**
 - What can we say about sources of biological and experimental variability? Uncertainty characterization applies in all layers: U(wet-lab), U(clinical), U(conceptual), U(trans), U(spec), U(in silico), and U(use cases [different individuals]).
- **A biomedical domain expert must be able to examine the model(s) and their simulation events (for the considered medical intervention) under different scenarios without needing computational expertise.**

Building Trustworthy Models

- Adopt “active learning” to improve model quality
 - data collection procedures specifically developed to reduce model uncertainty in an active manner
 - go beyond predictive validity
- Develop model evaluation criteria at the beginning of the model development process
- VV&UQ should be addressed in the context of a model’s use case
 - level of criticality of the clinical decision being made

So what can Multiscale Models do for Precision Medicine??



[Read/Purchase](#)

Toward Precision Medicine: Building a Knowledge Network for Biomedical Research and a New Taxonomy of Disease (2011)



Like

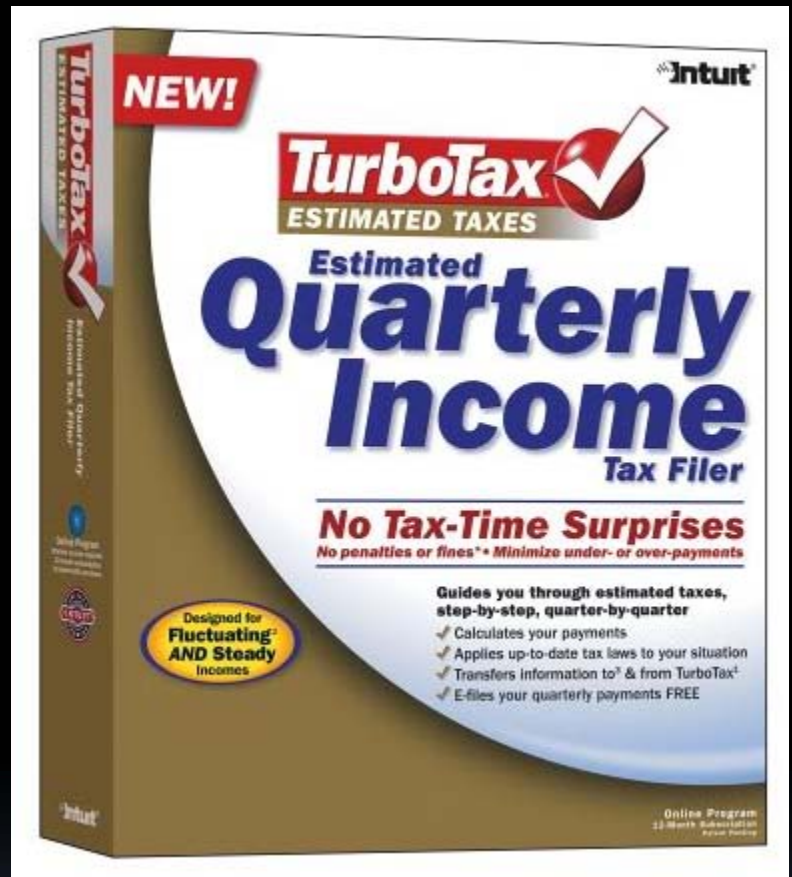
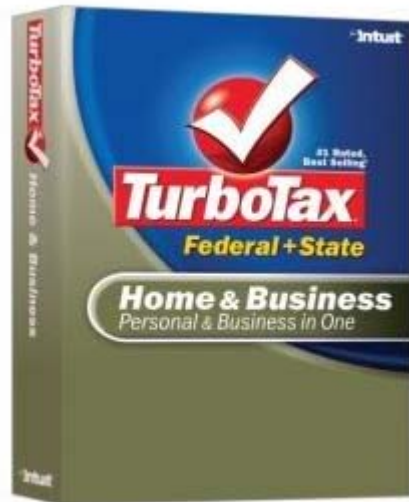


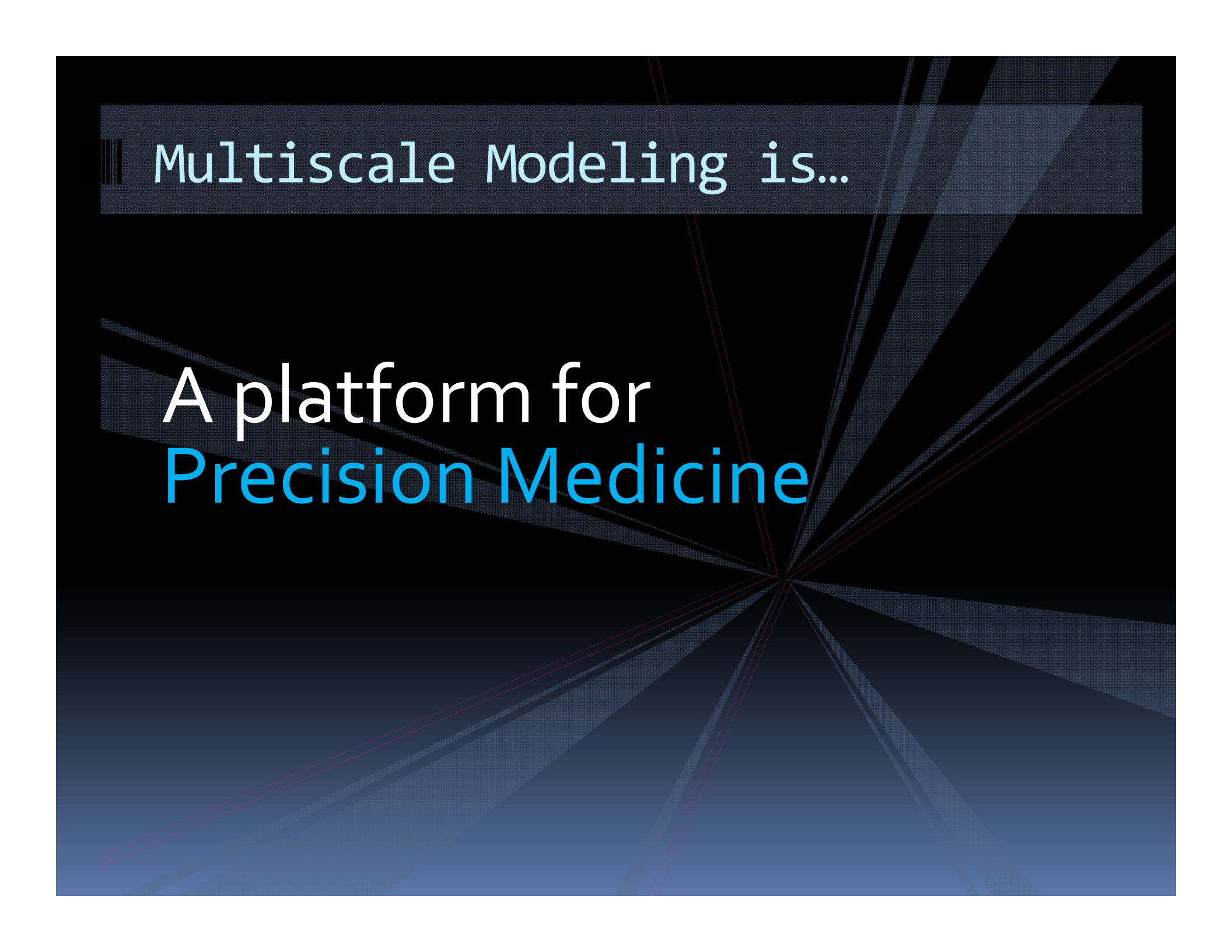
12 people like this. [Sign Up](#) to see what your friends like.

A new data network that integrates emerging research on the molecular makeup of diseases with clinical data on individual patients could drive the development of a more accurate classification of disease and ultimately enhance diagnosis and treatment. Recent advances in biomedical research have caused an explosion of data, offering the potential to develop a "new taxonomy" that defines disease based on underlying molecular and environmental causes, rather than on physical signs and symptoms. This report outlines how research and clinical data can be captured in a "knowledge network" that will be broadly accessible to researchers and clinicians. As well as improving health care, the new data network could also improve biomedical research by enabling scientists to access patient information through electronic health records, while still protecting patient rights.

The Ultimate Vision

- Model-driven, community-driven scientific discovery
 - Accelerated discovery
 - Prevalence of reproducible and reuseable models
- A “Turbo Tax” for science and discovery

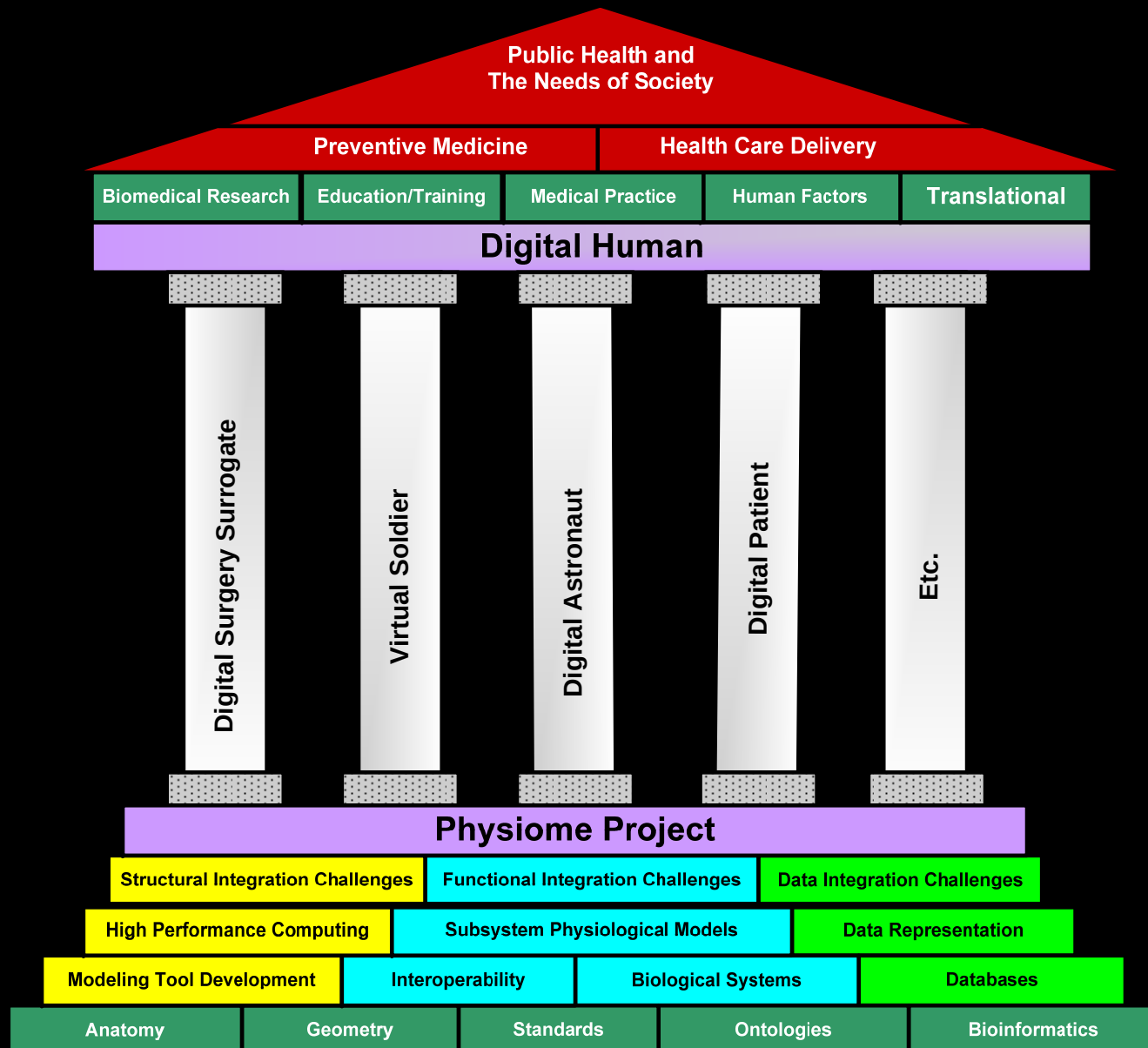




Multiscale Modeling is...

A platform for
Precision Medicine

The Present is Creating the Future



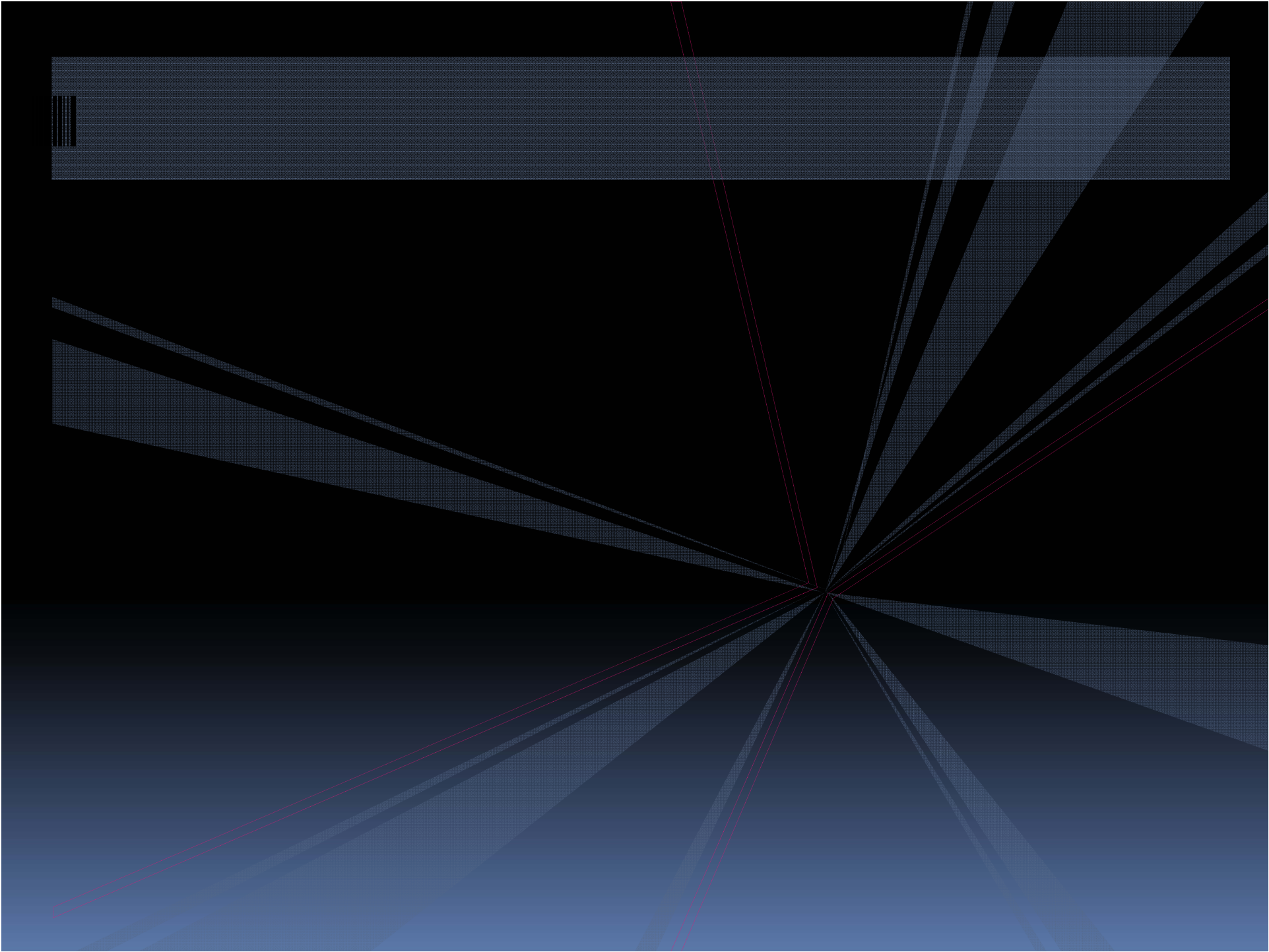
Courtesy of Ron White

どうもありがとう!

Grace C.Y. Peng

penggr@mail.nih.gov





CURRENT IMAG Funding Opportunity

PAR 11-203

Predictive Multiscale Models for Biomedical, Biological, Behavioral, Environmental and Clinical Research (Interagency U01)

- Promoting the next generation cutting edge multiscale models – **think out of the box**
- Participating Agencies: **NIH, NSF, DOE, FDA**
- 9 receipt dates until: **January 31, 2014**
- Cooperative Agreement allows investigators to contribute funded efforts to the MSM Consortium
- Requirements detailed in the FOA – **please read!**
 - Partnership Plan and MSM Consortium Plan

IMAG

PAR-11-203 Interests

- addressing **compelling** biological, biomedical, behavioral, environmental and clinical problems that require multiscale models to bring together different spatial and temporal scales within a specific field
- next generation multiscale models that **integrate between different fields** (e.g. cardiovascular and neuroscience) and predict integrated functions
- novel methods to **fuse data-rich and data-poor scales** to enable predictive modeling
- novel methods to **fuse biological and/or behavioral processes** and mechanisms to model outcomes as a result of various interventions
- **useable and reuseable** multiscale models that will be integrated and adopted into **model-poor fields** (e.g. tissue engineering, regenerative medicine, drug and gene delivery, preventive interventions)
- multiscale models strongly coupled with standardized protocols for **model-driven data collection**
- implementing **virtual clinical trials** with multiscale models to predict outcomes

IMAG

PAR-11-203 Interests

- problem-driven multiscale models that require **high performance computing** (NSF-OCI, DOE-BER)
- model predictions that drive a community of experimentalists towards **systematic testing and validation**
- predictive multiscale models that strongly **incorporate uncertainty quantification**
- mechanistic multiscale models that **bridge to the population level** to capture more clinical and biological realism for the population
- stochastic multiscale models that **characterize interactions between individual-level behaviors and group-, market-, or population-level outcomes**
- models to explore **underlying mechanisms** of individual-, community-, or **population-level preventive or therapeutic interventions**
- predictive multiscale models to **improve clinical workflow**, standard operating procedures, patient-specific modeling for diagnosis and therapy planning

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NIH Programs and Initiatives in Biomedical Informatics and Computational Biology (BICB)

Funding Categories
Funding Announcements

Broad-based BISTI initiatives

- BISTI Innovations in Biomedical Computational Science and Technology (R01) – [PAR-09-218](#) ; (R21) – [PAR-09-219](#); BISTI keeps a list of [R01 contact program staff](#) (A)
- BISTI Continued Development and Maintenance of Software (R01) – [PAR-11-028](#) (A)
- BISTI Innovations in Biomedical Computational Science and Technology Initiative (SBIR [R43/R44]) – [PAR-09-220](#) ; (STTR [R41/42])– [PAR-09-220](#); BISTI keeps a list of [SBIR/STTR contact program staff](#) (A)
- Collaborations with National Centers for Biomedical Computing (R01) – [PAR-08-184](#) ; (R21) – [PAR-08-183](#) (A)

- BISTI Continued Development and Maintenance of Software (R01) – [PAR-11-028](#) (A)
- BISTI Innovations in Biomedical Computational Science and Technology Initiative (SBIR [R43/R44]) – [PAR-09-220](#) ; (STTR [R41/42])– [PAR-09-220](#); BISTI keeps a list of [SBIR/STTR contact program staff](#) (A)
- Collaborations with National Centers for Biomedical Computing (R01) – [PAR-08-184](#) ; (R21) – [PAR-08-183](#) (A)

Broad-based or multi Institute Programs and Initiatives

- Research Project Grant (Parent R01) – [PA-10-067](#) The Parent R01 is used for the majority of applications that go to

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