AI FOR SCIENCE TOWN HALL

AI for Science Grand Challenges

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AI and Biology

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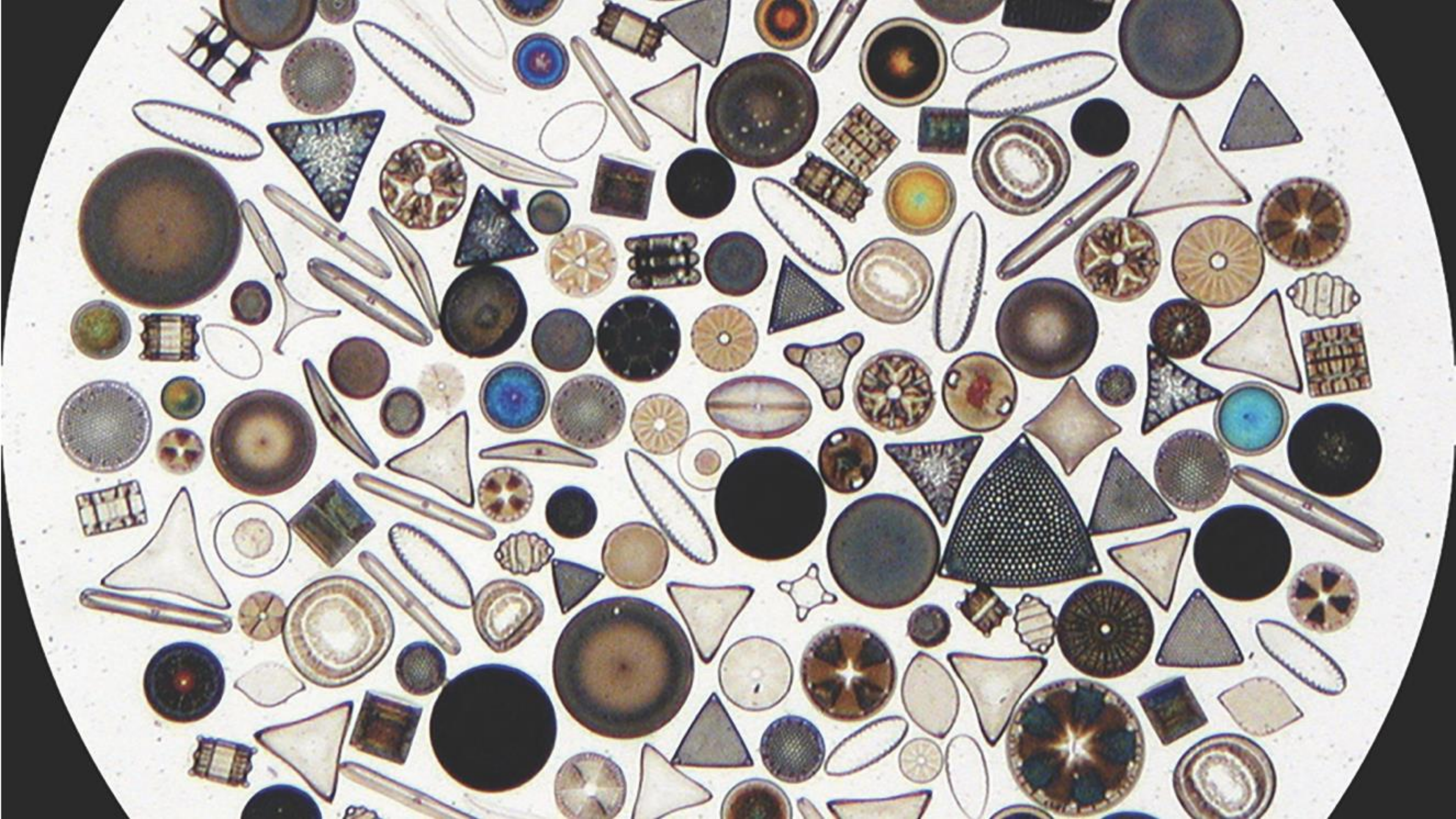
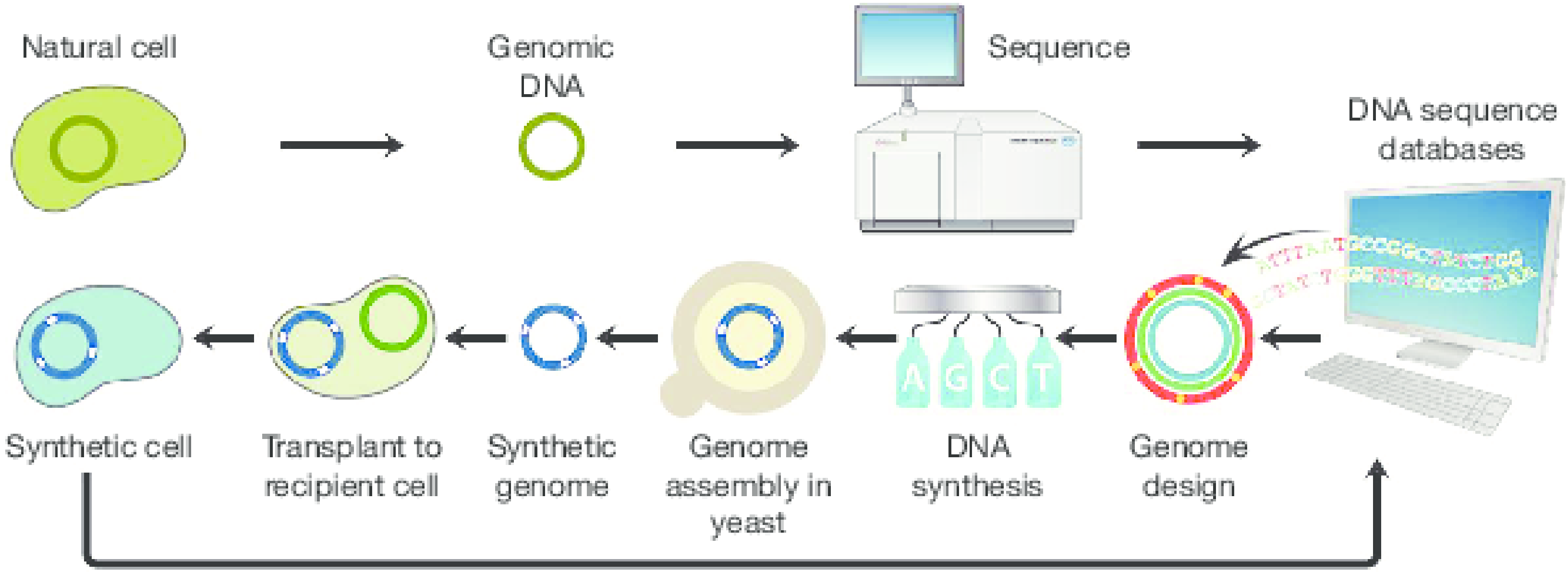


Use AI to Accelerate Synthetic Biology

- **AI to predict the relationship between Genotypes and Phenotypes**
  - Today ML can predict antibiotic resistance from genomes without culturing the organism as accurately as we can measure resistance in the lab
- **ML to predict protein function from protein sequence**
  - Today DL can predict protein structure from sequence (DeepMind, TTIC, etc.)
- **Generative models to design biosynthetic pathways**
  - Today ML can predict metabolic pathways from genomes
- **Generative models to compose collections pathways into subsystems**
- **Generative models to translate from collections of functions to a set of modules**
- **Models to wrap biological modules with regulation and signaling systems**
- **Seq2seq models to translate functional blocks into genome sequences**
- **AI to control the routine fabrication and synthesis of novel whole organisms**

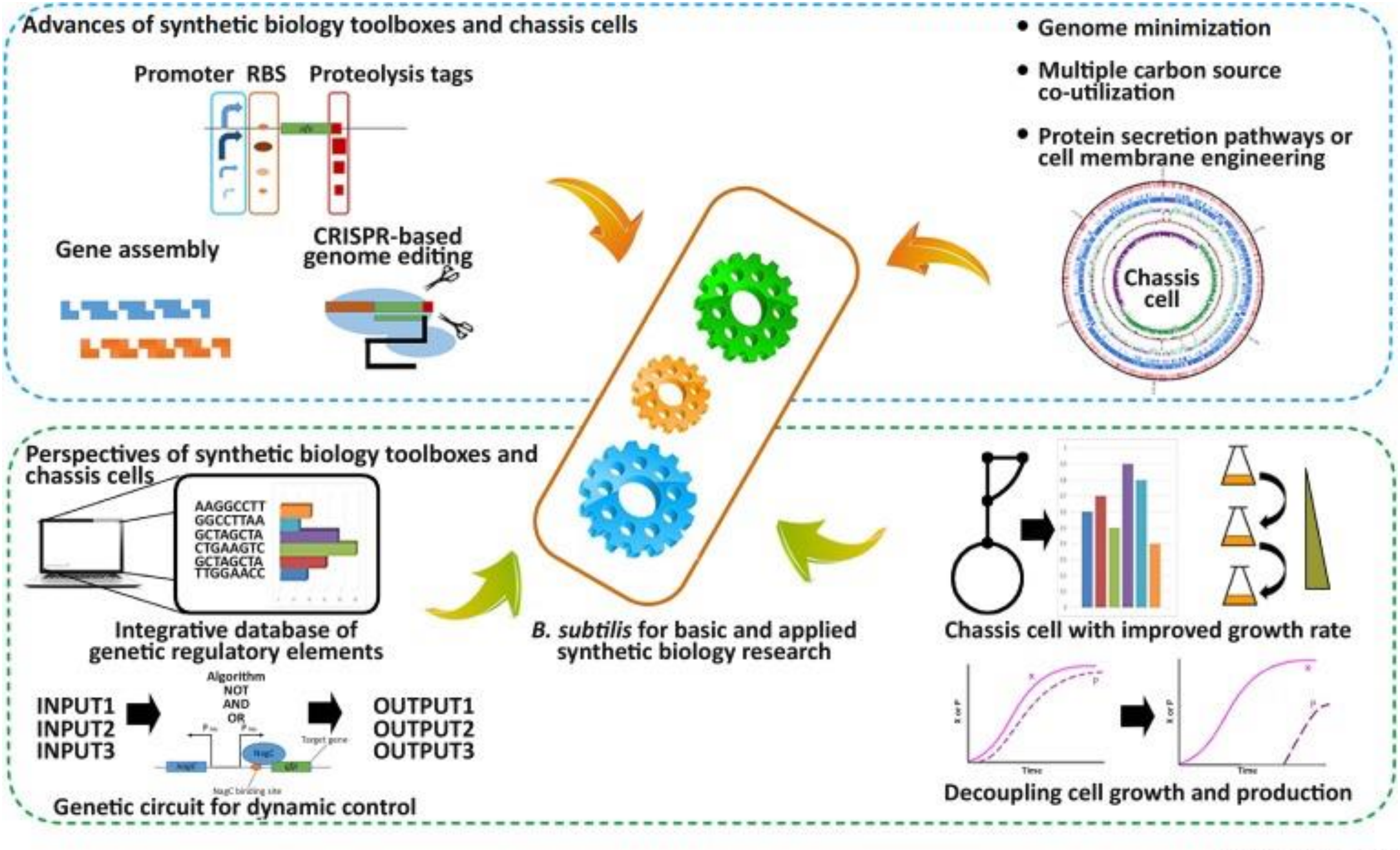
Building the Database to Support BioDesign



Today we have >300,000 genomes >100,000 metagenomes

In ten years we could have > 10,000,000 genomes >1,000,000 metagenomes

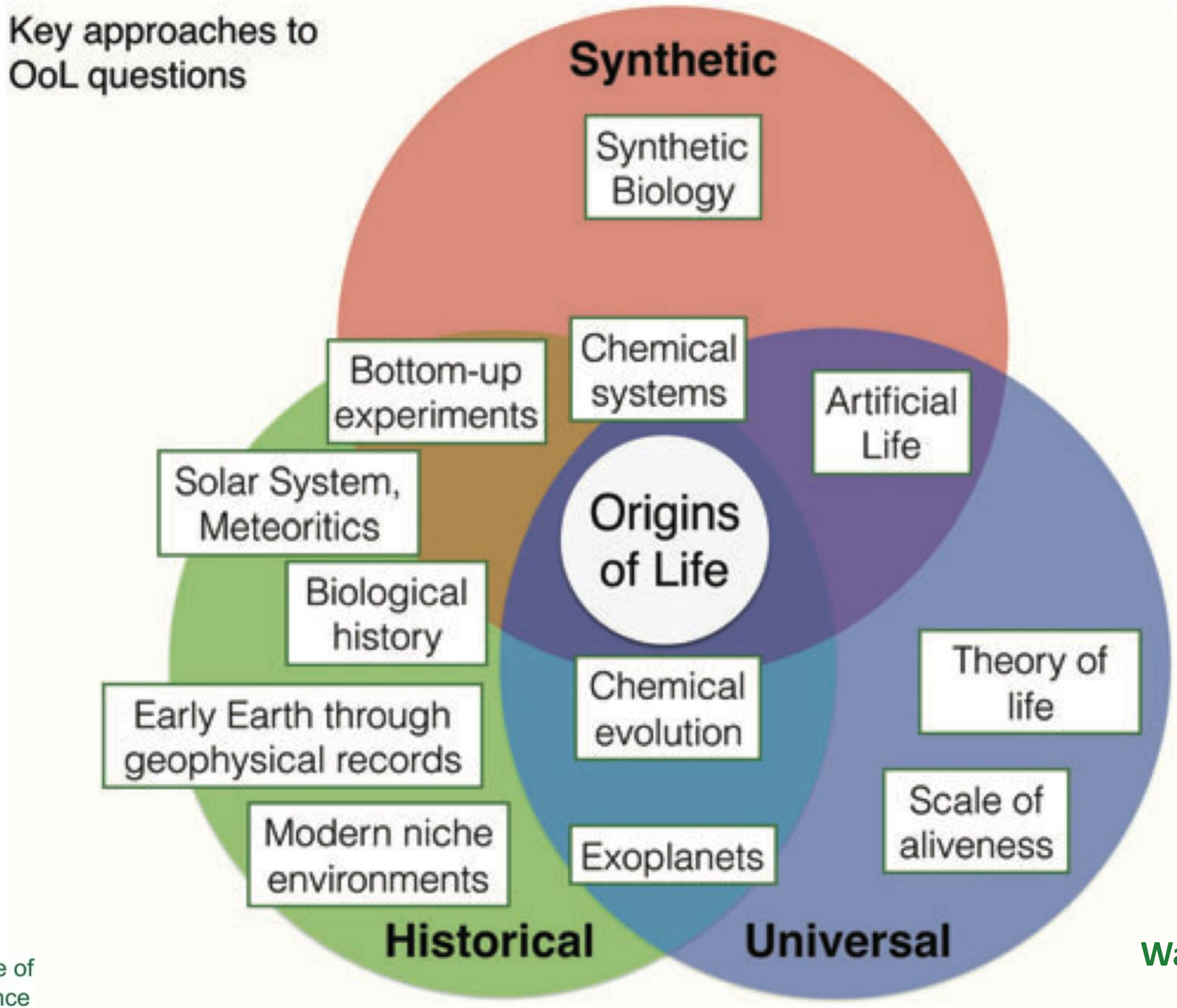
Food for Models!

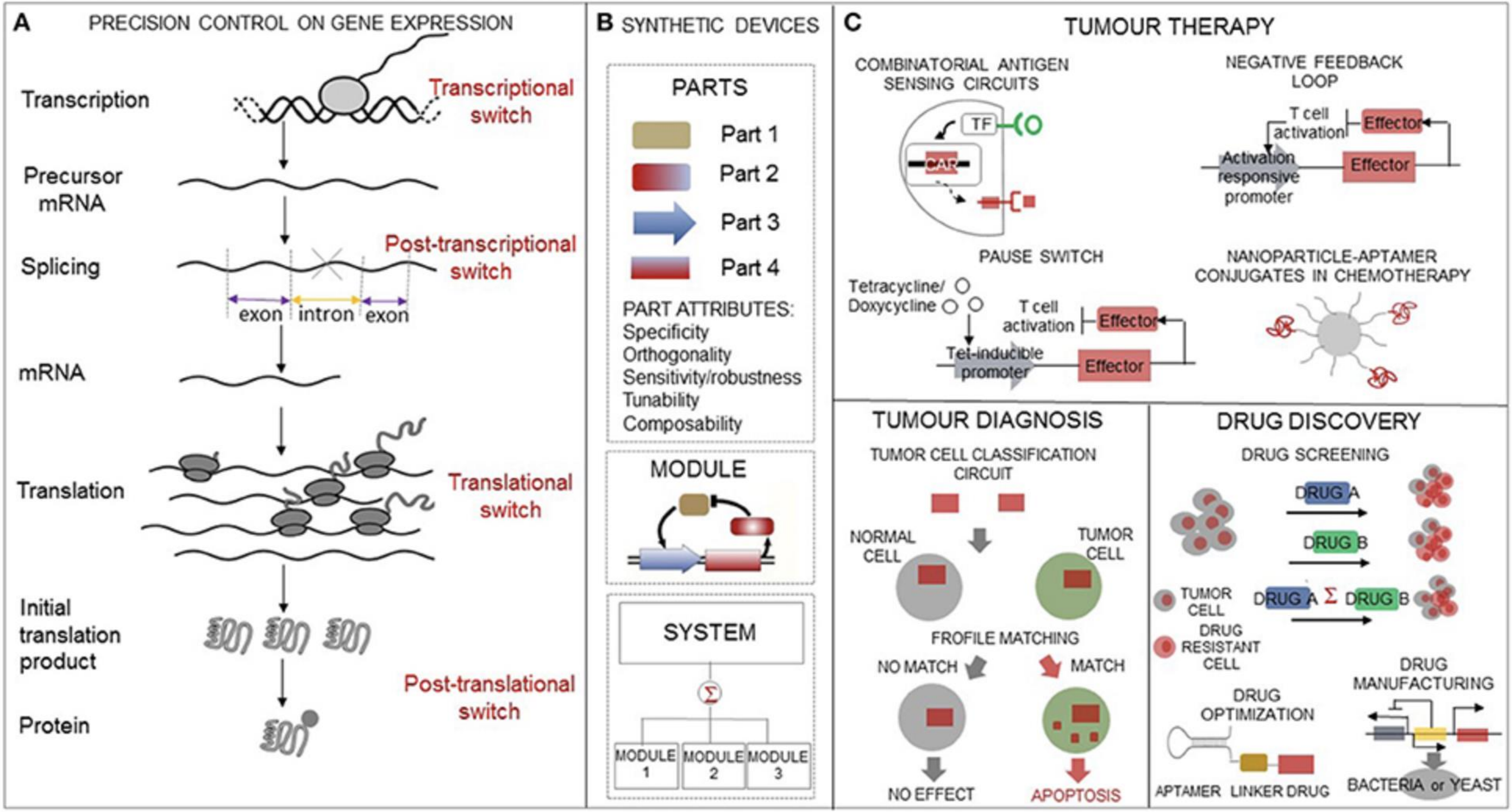


Trends in Biotechnology

With a robust biodesign capability we could…

- Replace chemical factories with small safe portable biomanufacturing
- Democratize and accelerate drug development
- Produce novel food grade protein and fiber sources
- Produce biological carbon capture systems
- Produce designer polymers that are environmentally benign
- Harness bespoke biological systems for water purification
- Integrate 3d printable bioinks with biological computing and control to produce new types of smart matter

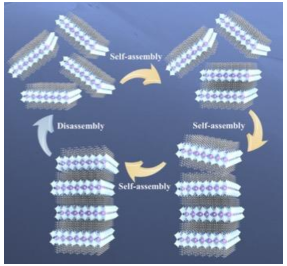

Key approaches to
OoL questions
Synthetic
Synthetic Biology
Chemical systems
Bottom-up experiments
Artificial Life
Solar System, Meteoritics
Origins of Life
Biological history
Chemical evolution
Theory of life
Early Earth through geophysical records
Modern niche environments
Exoplanets
Scale of aliveness
Historical
Universal


A PRECISION CONTROL ON GENE EXPRESSION
Transcription
Transcriptional switch
Precursor mRNA
Splicing
Post-transcriptional switch
exon
intron
exon
mRNA
Translation
Translational switch
Initial translation product
Post-translational switch
Protein
B SYNTHETIC DEVICES
PARTS
Part 1
Part 2
Part 3
Part 4
PART ATTRIBUTES:
Specificity
Orthogonality
Sensitivity/robustness
Tunability
Composability
MODULE
SYSTEM
Σ
MODULE 1
MODULE 2
MODULE 3
C
TUMOUR THERAPY
COMBINATORIAL ANTIGEN SENSING CIRCUITS
TF
CAR
NEGATIVE FEEDBACK LOOP
T cell activation
Effector
Activation responsive promoter
Effector
PAUSE SWITCH
Tetracycline/ Doxycycline
T cell activation
Effector
Tet-inducible promoter
Effector
NANOPARTICLE-APTAMER CONJUGATES IN CHEMOTHERAPY
TUMOUR DIAGNOSIS
TUMOR CELL CLASSIFICATION CIRCUIT
NORMAL CELL
TUMOR CELL
FROFILE MATCHING
NO MATCH
MATCH
NO EFFECT
APOPTOSIS
DRUG DISCOVERY
DRUG SCREENING
DRUG A
DRUG B
DRUG A Σ DRUG B
TUMOR CELL
DRUG RESISTANT CELL
DRUG OPTIMIZATION
APTAMER
LINKER
DRUG
DRUG MANUFACTURING
BACTERIA or YEAST

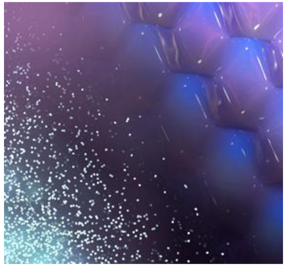
AI at the User Facilities

DOE facilities are the backbone of experimental science

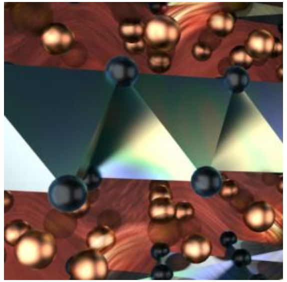
X-rays | Neutrons | Nano



Nanomaterials



Superconductors



Superionic crystals

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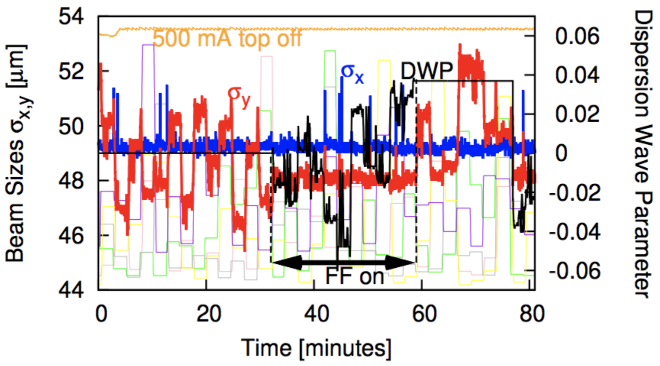
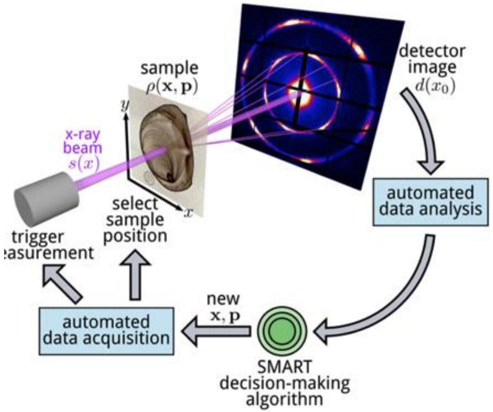
Three AI Problems in Facilities

Accelerator control



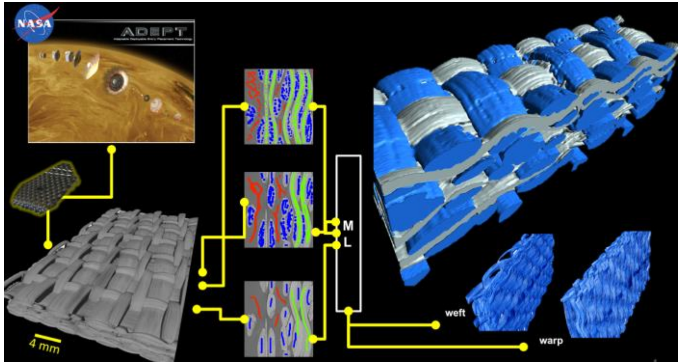
Improve beam stability

Autonomous experiments



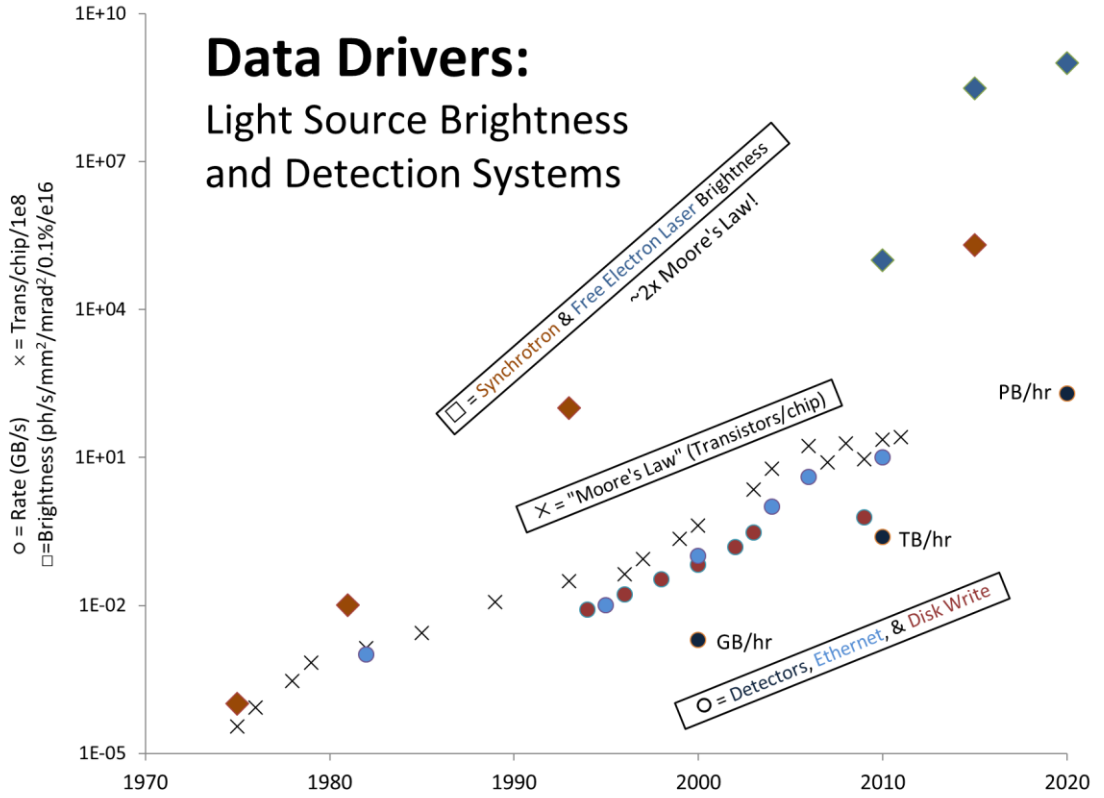
Improved efficiency in beamlines

AI-based Data Analysis



Automated data reduction

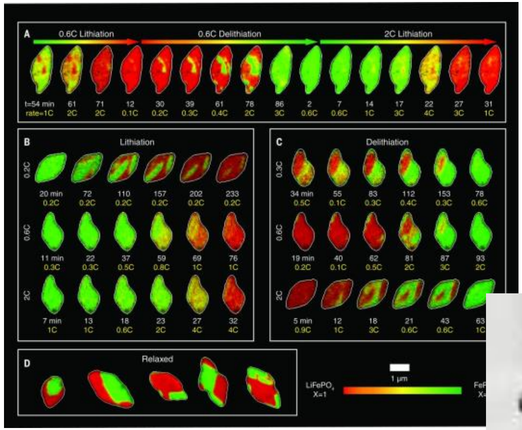
Data Growth will drive AI at the Edge

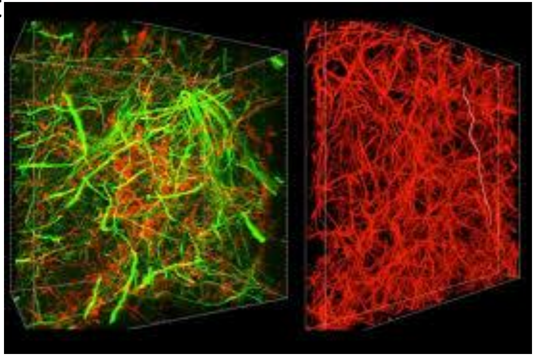


source: D. Parkinson, LBNL

Grand Challenges across Length scales and Under Extreme Environments

Predict, mitigate and prevent harmful algae blooms?





Understand the brain

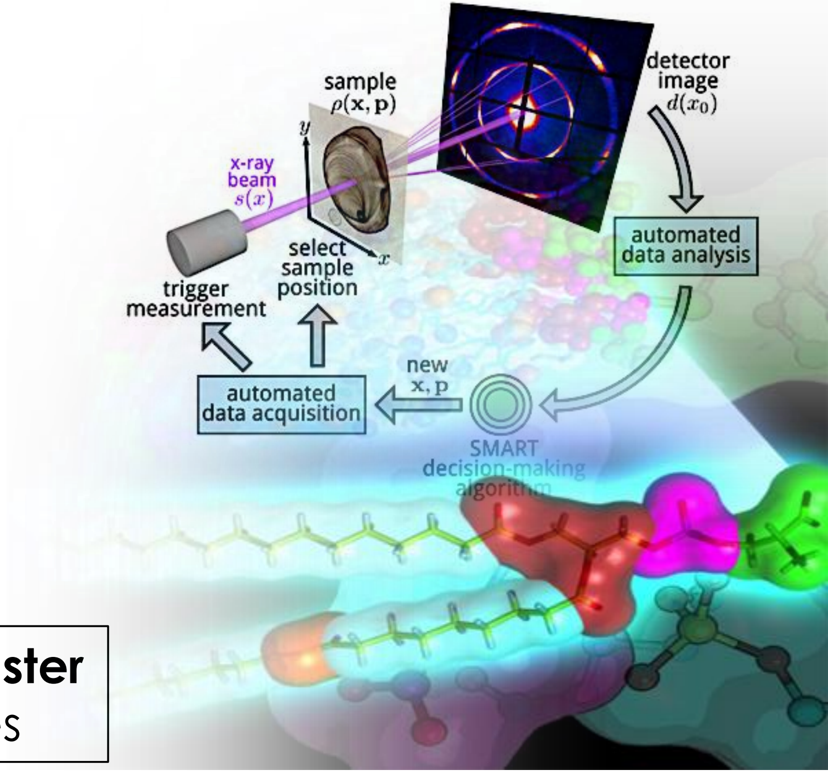
Improve capacity of rechargeable batteries

AI and Materials

Transformative advances are possible

On-the-fly materials/chemical synthesis

- Requires autonomous-smart experiments and simulations
  - needs a new class of machine learning algorithms that continually learn and update their predictions based on new data sources, encode physical constraints/laws and models, and learn to estimate fidelity



Delivering materials/chemical ~**1000x faster** and with desired performance/properties

For example – synthesize a new quantum material

- Using Pulsed Laser Deposition (PLD) use high-power lasers to vaporize a sample (the source of the elements) inside a vacuum reaction chamber to produce elements in a vapor plume. ‘
- The vapor plume then deposits on a substrate where it is templated and the materials grows (very fast process).
- The growth and elemental stoichiometry depends on the chamber temperature, rate of vaporization, and deposition time.
- Measure optical properties of the plume in-situ and control the processing variables - if correlations could be found/controlled via AI.

AI and Cosmology

Universe: The Movie

Reconstruct the past from the Big Bang until today and predict the future of our visible Universe, from the largest scales down to our own galaxy.

Use all existing data (galaxy positions, stellar mass, velocities, dark matter maps, gas distribution, tSZ, kSZ, X-ray).

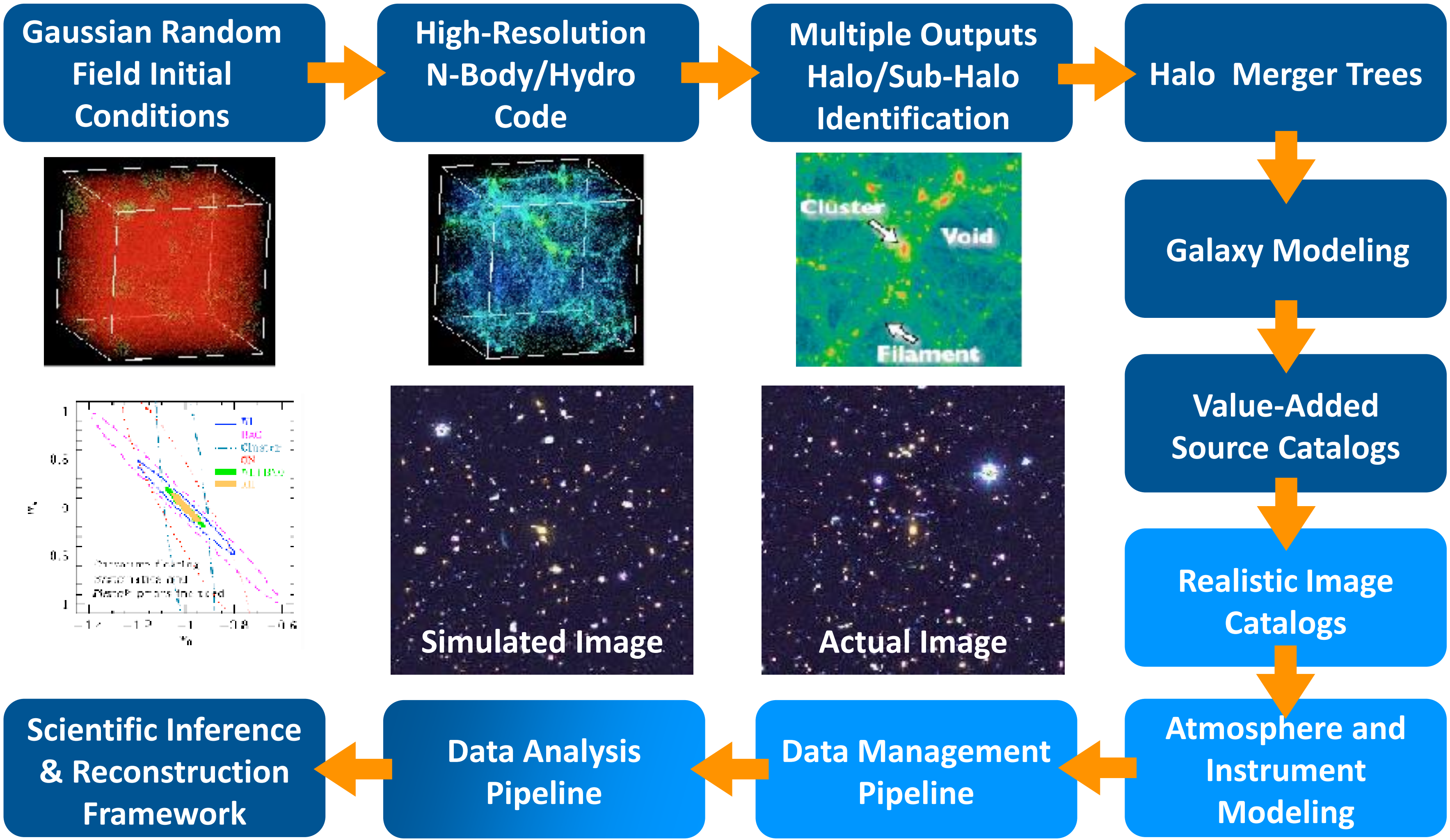
What is dark energy? What is its density evolution in time? What is the nature of dark matter? Did inflation happen?

Provide tightest possible constraints on fundamental physics questions by solving optimal inference problem.

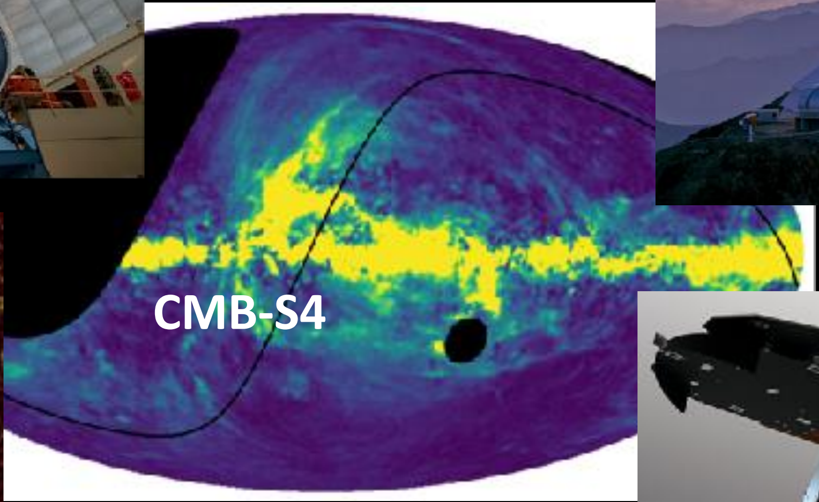
Universe: The Movie

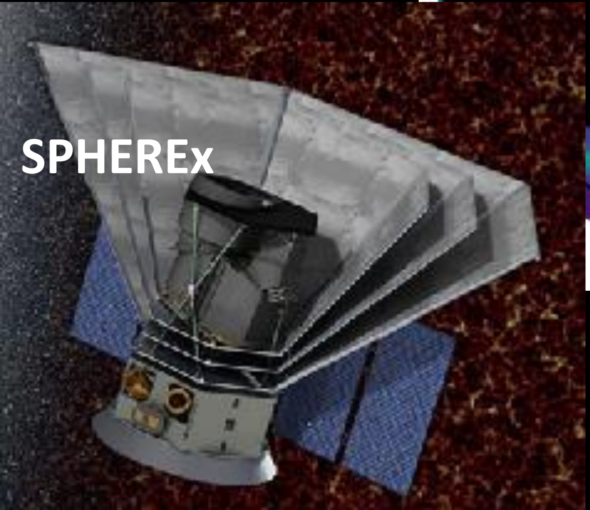
Brought to you by AI

- GANs for image emulation
- GP and DL-based emulators for summary statistics
- CNN-based image classification
- AI-based photometric redshift estimation
- AI methods for inference and reconstruction


Gaussian Random Field Initial Conditions
High-Resolution N-Body/Hydro Code
Multiple Outputs Halo/Sub-Halo Identification
Halo Merger Trees
Cluster
Void
Filament
Galaxy Modeling
Value-Added Source Catalogs
Realistic Image Catalogs
Simulated Image
Actual Image
Atmosphere and Instrument Modeling
Data Management Pipeline
Data Analysis Pipeline
Scientific Inference & Reconstruction Framework

The next decade of Sky Surveys

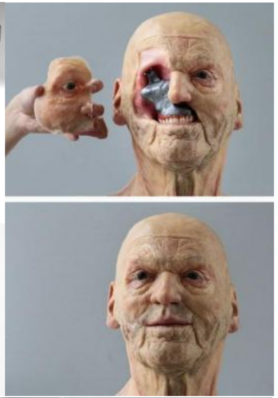




AI in Manufacturing

Zero waste on-demand bespoke manufacturing

- Optimization of material (polymer, ceramic, composite, metal, or hybrid), shape, topology, and performance (strength, lifetime) given a functional requirement
- Requires advances in
    - science (fundamental understanding of materials and manufacturing processes),
    - engineering (manufacturing systems, sensors),
    - computing (both a priori optimization and real-time control)



Ultimately, “replicators”

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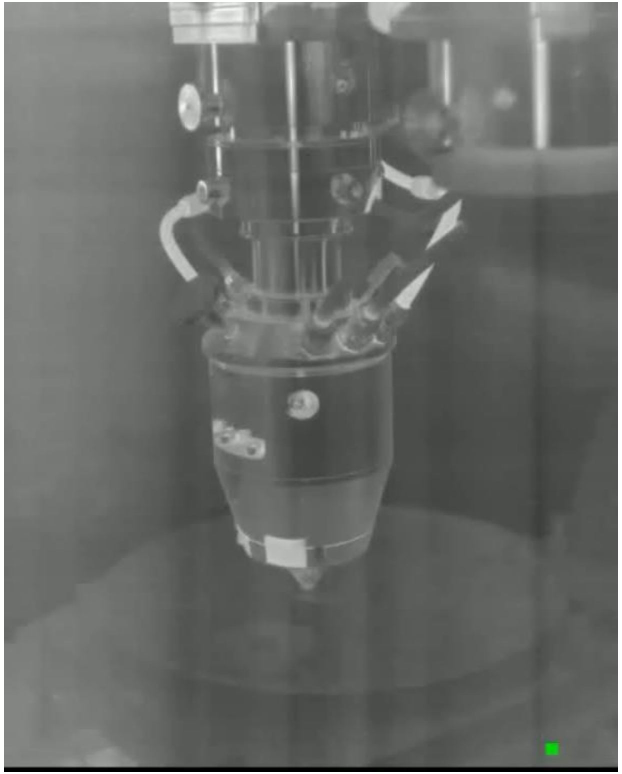
Cradle-to-grave system state awareness

- Extension of “digital twin” concept
- Aerospace, civil, mechanical, chemical, nuclear engineering, stockpile stewardship, etc.
- Complete knowledge of a system throughout its lifecycle
  - Design system functionality and monitoring in at the material and manufacturing level
  - Monitor, control and assess in-service system condition (Structural Health Monitoring)
  - Intelligent Life Extension & System Retirement (Structural Health Monitoring/Damage Prognosis/Probabilistic risk assessment)
- Requires advances in sensor technology, understanding of ageing and failure modes, data acquisition and management, cybersecurity, and AI integration

Enable adoption of reliable, low-cost clean nuclear energy

- Leverage latest innovations in materials, manufacturing, and machine learning to enable rapid and economical production of nuclear energy systems
  - not limited by the constraints of conventional manufacturing and pre-1970s materials,
  - meet or exceed safety standards
- Printing a reactor
  - New materials, additive manufacturing, embedded sensors and controls, integrated design and performance prediction, workforce development



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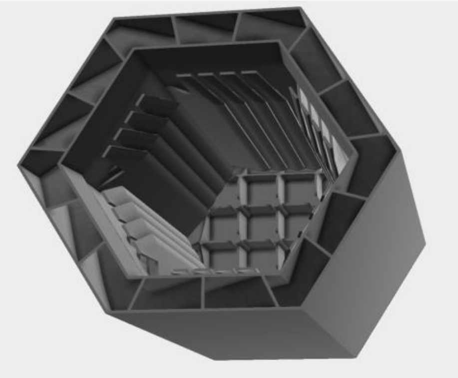
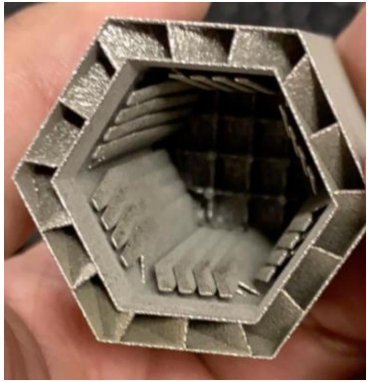
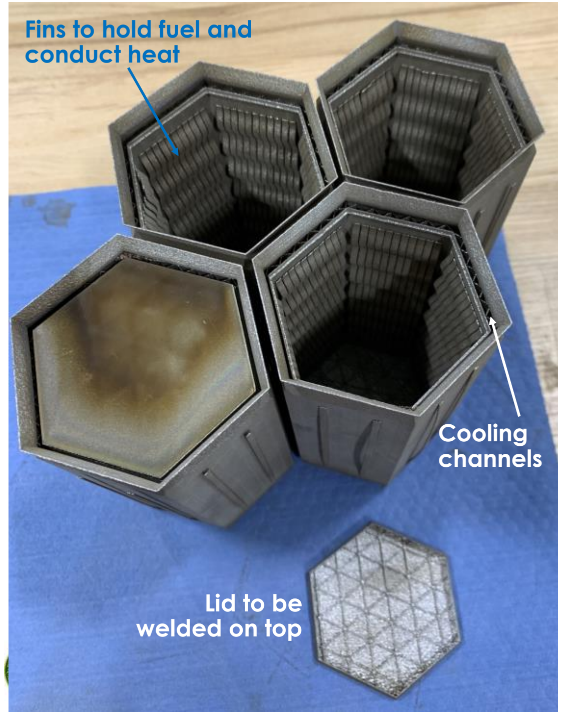
Printed reactor components



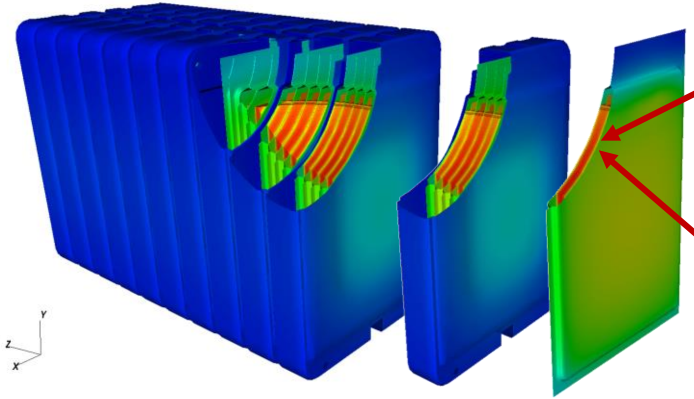




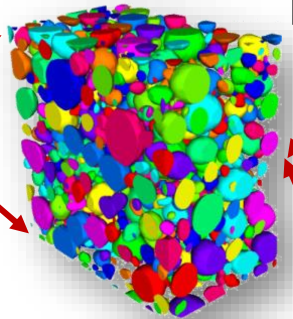
Accelerate adoption of electric vehicles and renewable energy through improved batteries

- 3-5 year priorities
  - Charge a 1000-cycle, 15-year lifetime, 250-Wh/kg Li-ion battery to 80% in 10-15 min.
  - Understand ageing - electrode / electrolyte interfaces and degradation
- 10-15 year priorities
  - Fundamental understanding of solid-electrolyte interphase (SEI) stability
  - Beyond Li-ion: higher energy density, calendar and cycle life

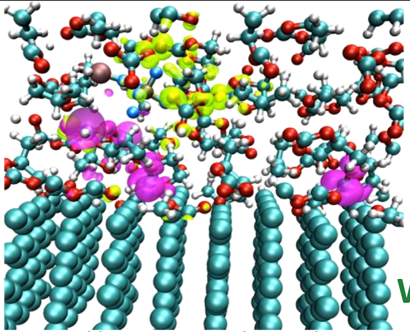
Leverage AI to bridge atomistic to macroscale properties, behavior, response



https://vibe.ornl.gov/



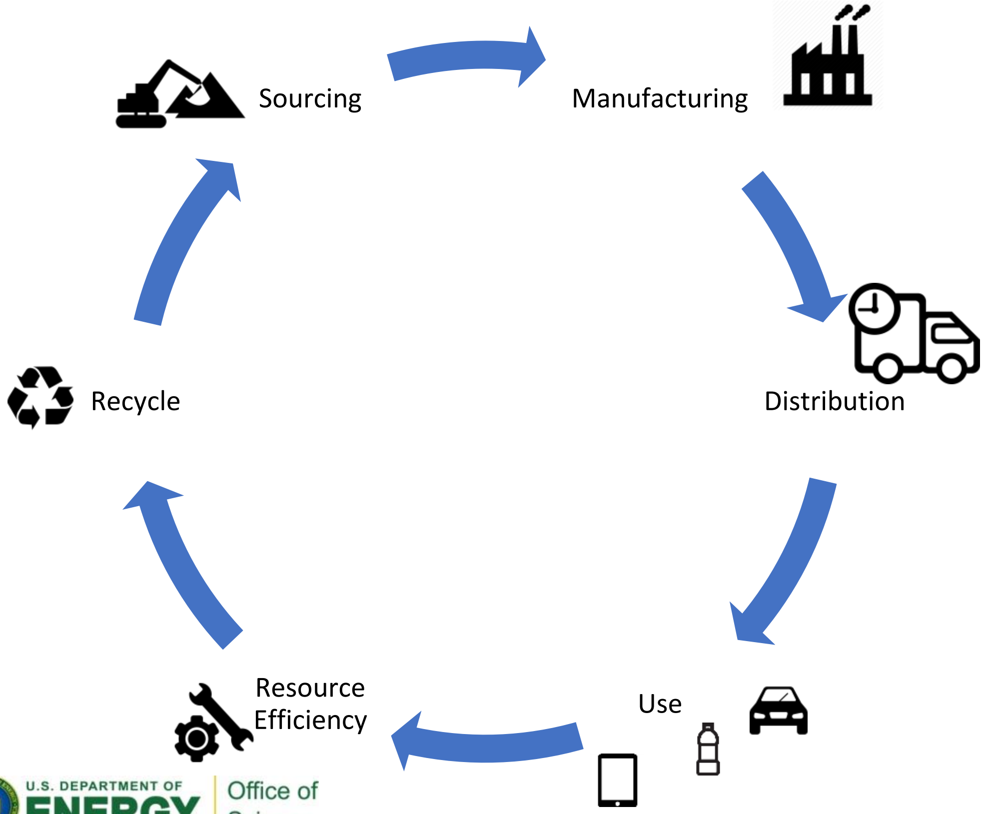
https://www.sandia.gov/~sarober/research.html



https://qsg.llnl.gov/node/40.html

Washington DC Town Hall
October 22-23

Enable transition to a circular economy



By 2050, the world's population will likely pass 10 billion.

As the earth's raw materials are not limitless, and global labor and the costs for these materials are on the rise, new solutions are needed to mitigate this emerging challenge.

Circular Economy business opportunities provide a way for manufacturing to grow and diversify under these pressures.

AI and Cities

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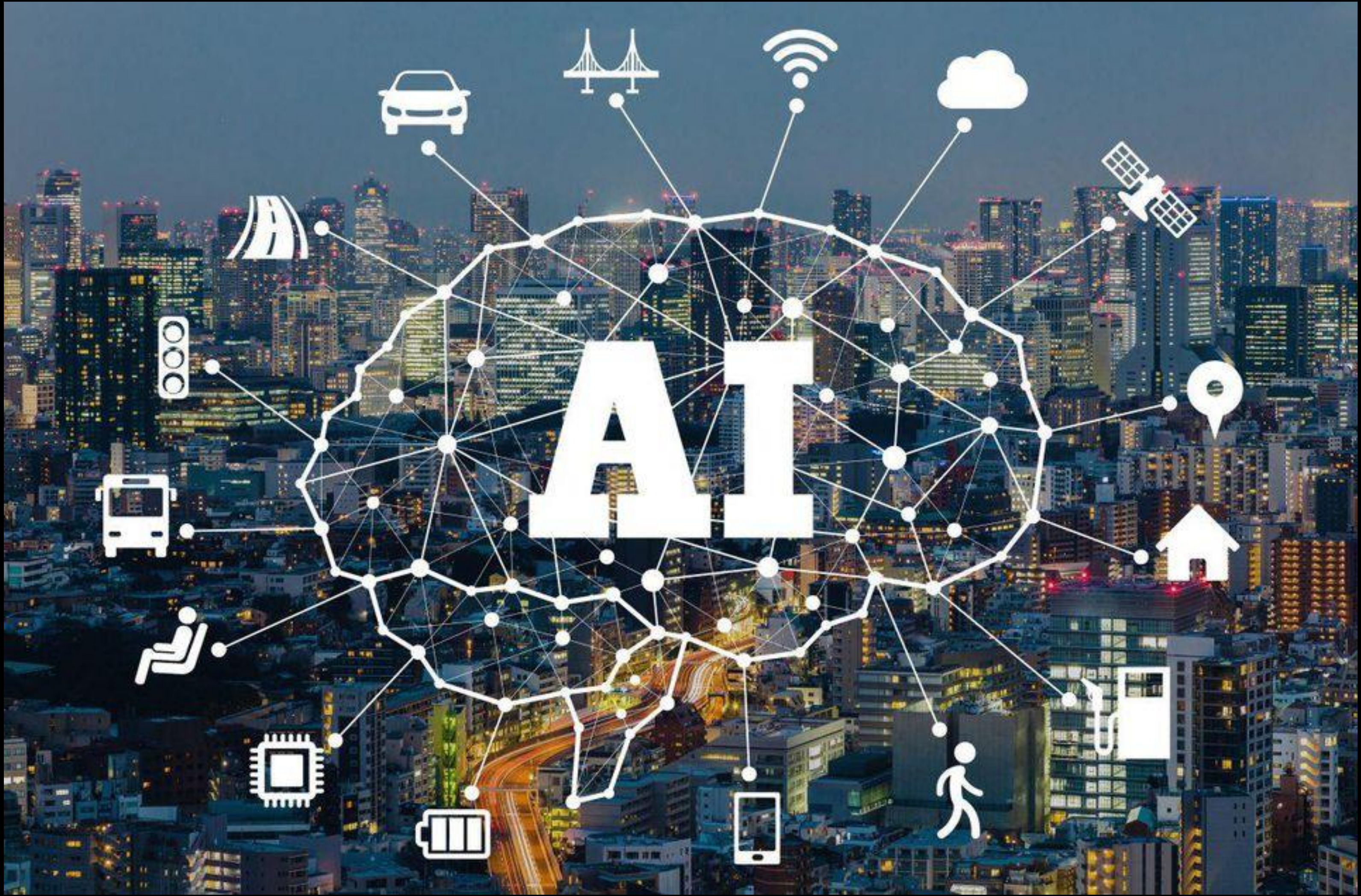
AI

80% of the population in developed countries is expected live in cities by **2050**

By **2025**, smart cities are expected to have a market value of more than **$2 trillion**

AI will play a role in such areas as:
smart parking, smart mobility, smart grid, adaptive signal control, waste management

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Other than AI, smart cities will rely upon:
robotics, ADAS, distributed energy generation

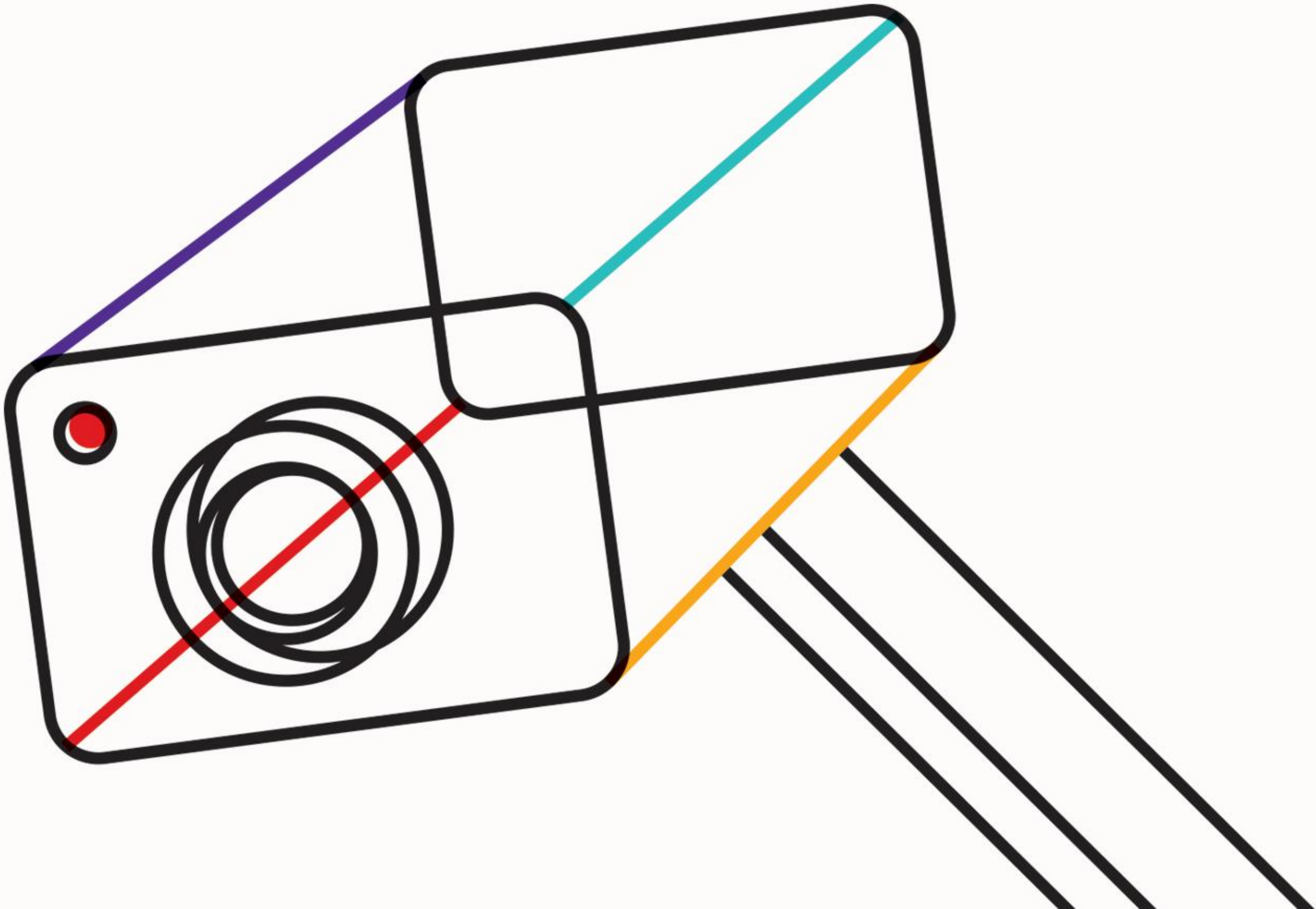
Edge Computing and Sensing

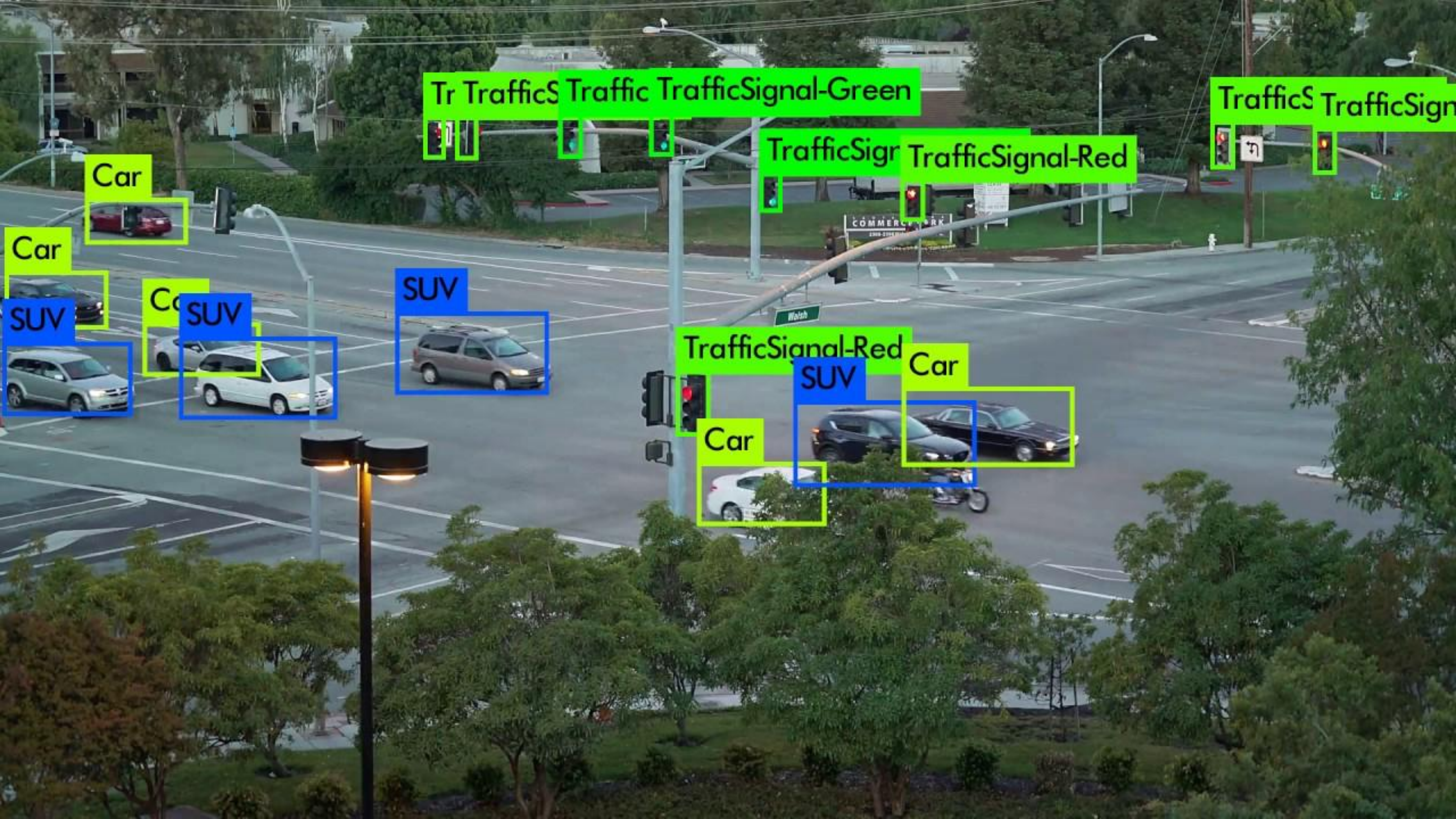
ARRAY OF THINGS


SAFETY
Soldering Station

AI for Smart Cities

- Improve quality of life and equality of opportunity
- Optimize mobility, safety, energy, and security
- Improve citizen engagement in civic life
- Increase information sharing and awareness
- Decrease environmental impact of cities
- Improve economic development
- Improve government services while ensuring freedoms





Tr
TrafficS
Traffic
TrafficSignal-Green
TrafficS
TrafficSign
TrafficSign
TrafficSignal-Red
Car
Car
SUV
Co
SUV
SUV
TrafficSignal-Red
SUV
Car
Car
COMMERC
Walsh


109,62,158,144
413,71,444,167
648,199,693,313

AI Revolution

- **Learned Models Replace Data**
- **Experimental Discovery Refactored**
- **Questions Pursued Semi-Autonomously**
- **Simulation and AI Merge**
- **Theory Becomes Data**
- **AI Laboratories**

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Discussion and Questions