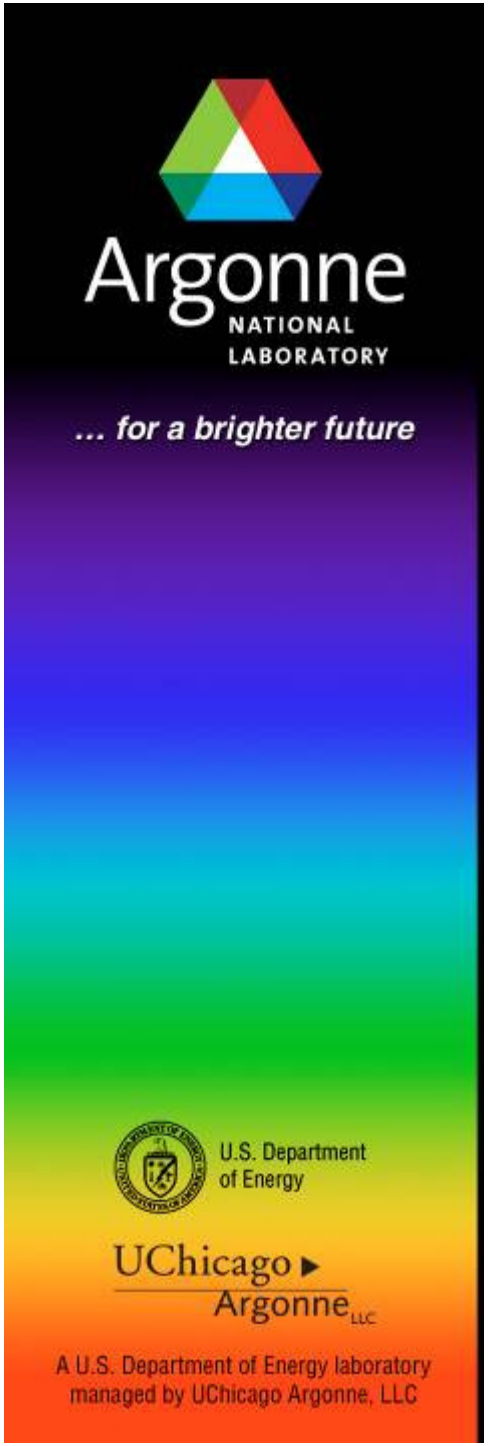


System Level Science and System Level Models

Ian Foster

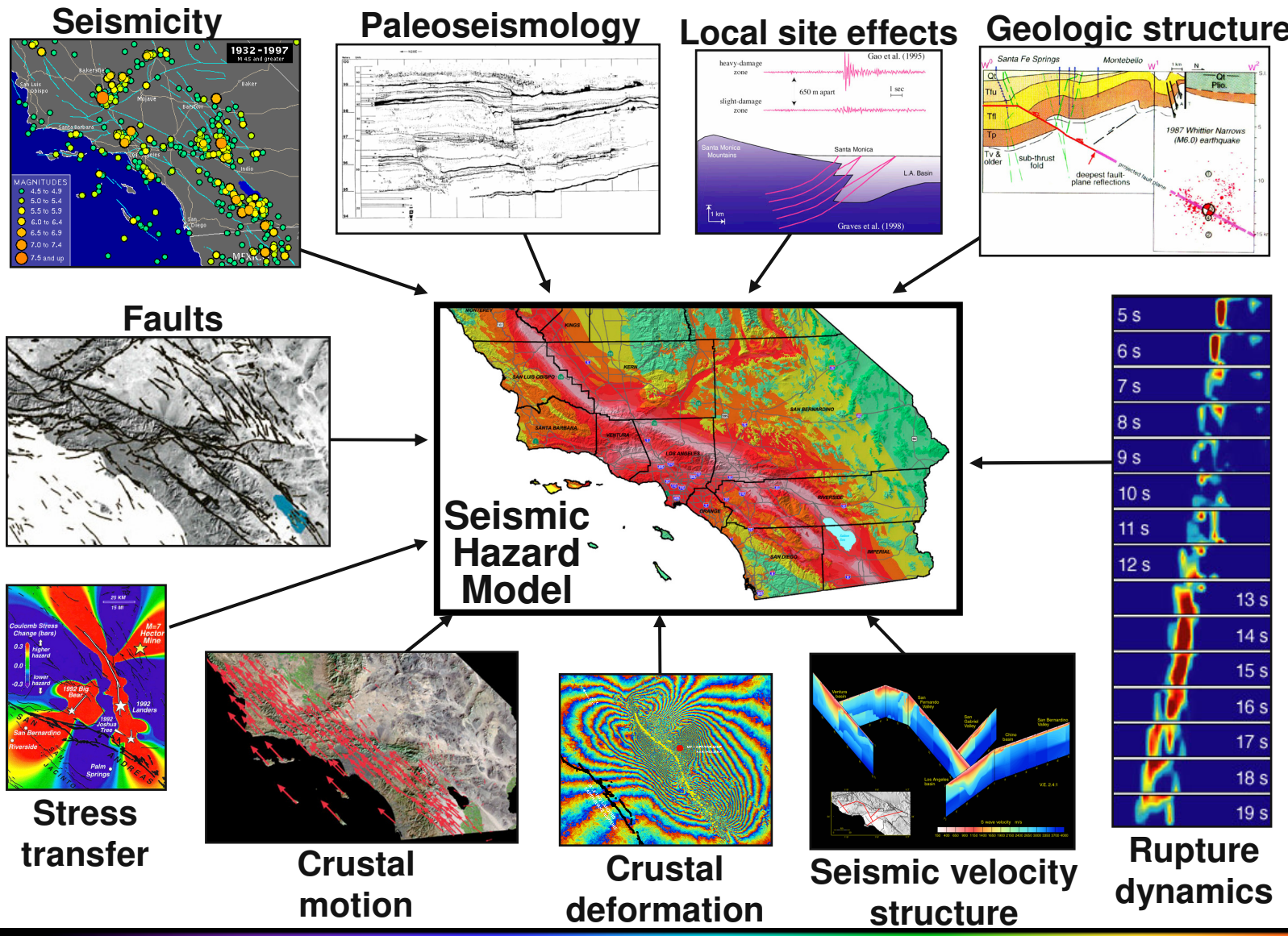
Argonne National Laboratory
University of Chicago

Improving IAM Representations of a Science-Driven Energy Future, **Snowmass, August 1-2, 2007**
Panel on "Alternative Modeling Perspectives: Challenges and Opportunities in Modeling Innovation, From Macro to Micro"

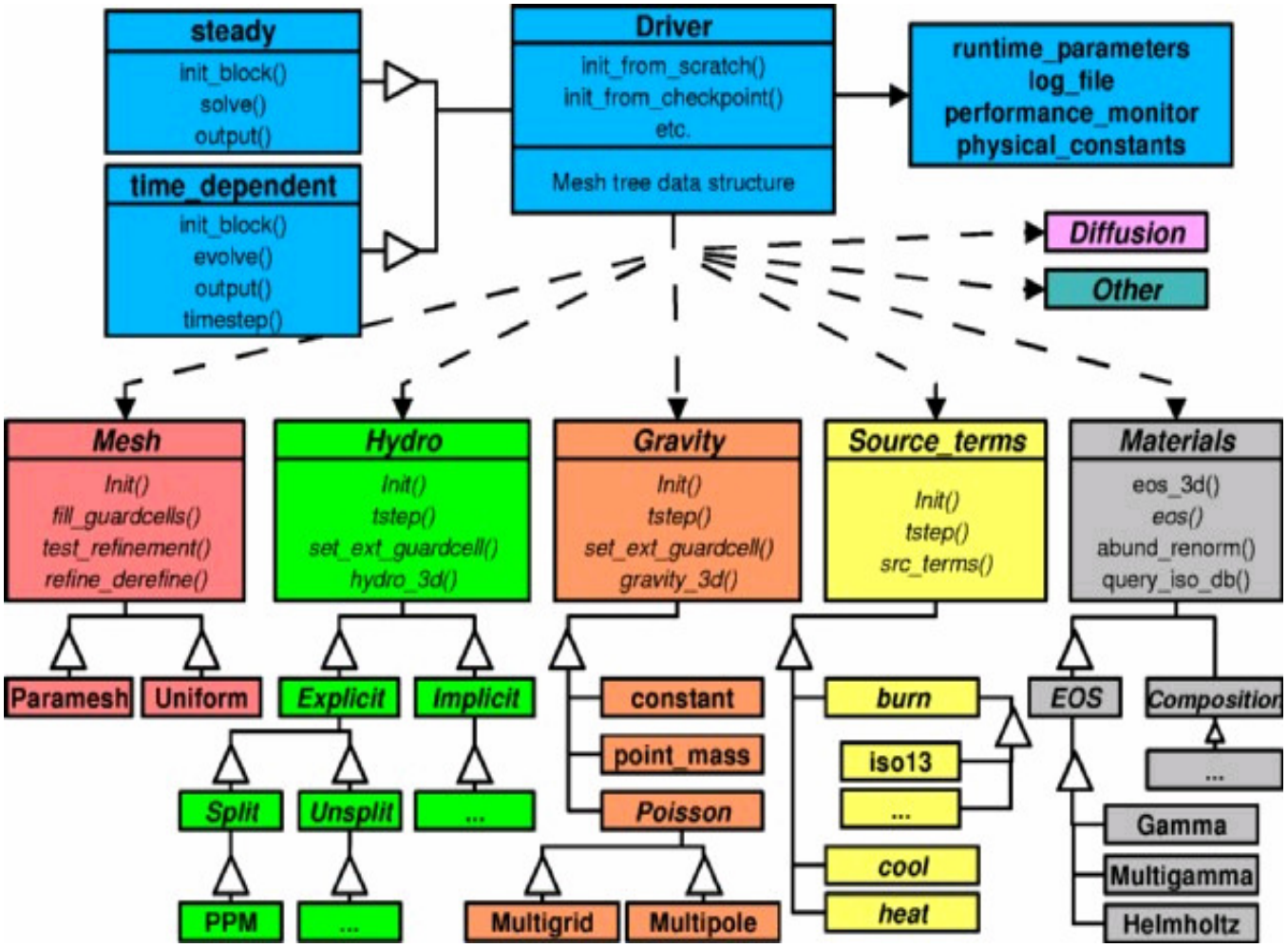
System Level Science

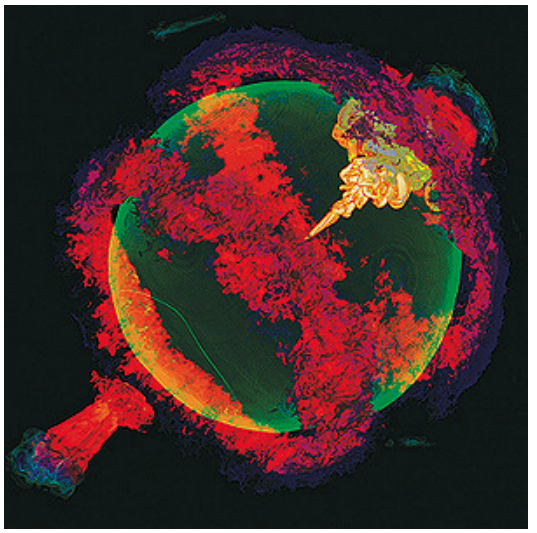
- Understanding in context
  - Move focus beyond individual phenomena
  - Understand how components interact and interrelate
- Characteristics
  - End-to-end
  - Multi-disciplinary, multi-phenomena
  - Alternative approaches for each component
  - Often need to integrate rich data sources
  - Seek to answer many different types of questions

Seismic Hazard Analysis (T. Jordan et al., SCEC)

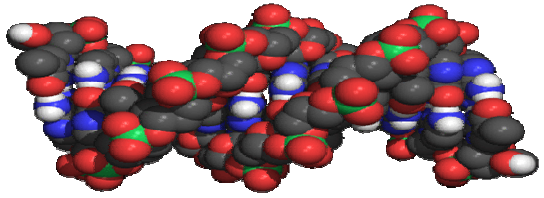


Astrophysics: The FLASH Code (U.Chicago)



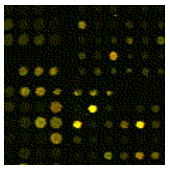


Systems Biology



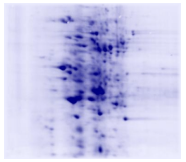
DNA (storage)

Transcription



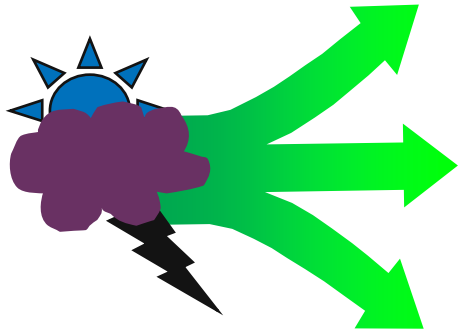
Translation

Proteins



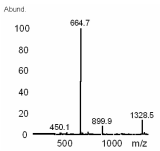
Proteomics

Gene Expression

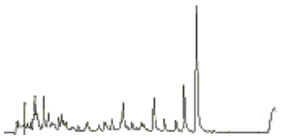


Environment

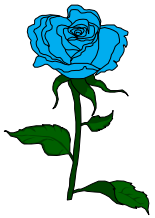
Biochemical Circuitry

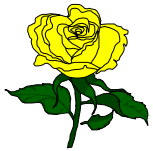


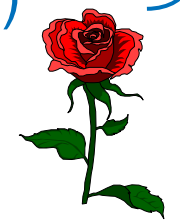
Metabolomics



Phenotypes (Traits)







Adapted from
Bruno Sobral VBI

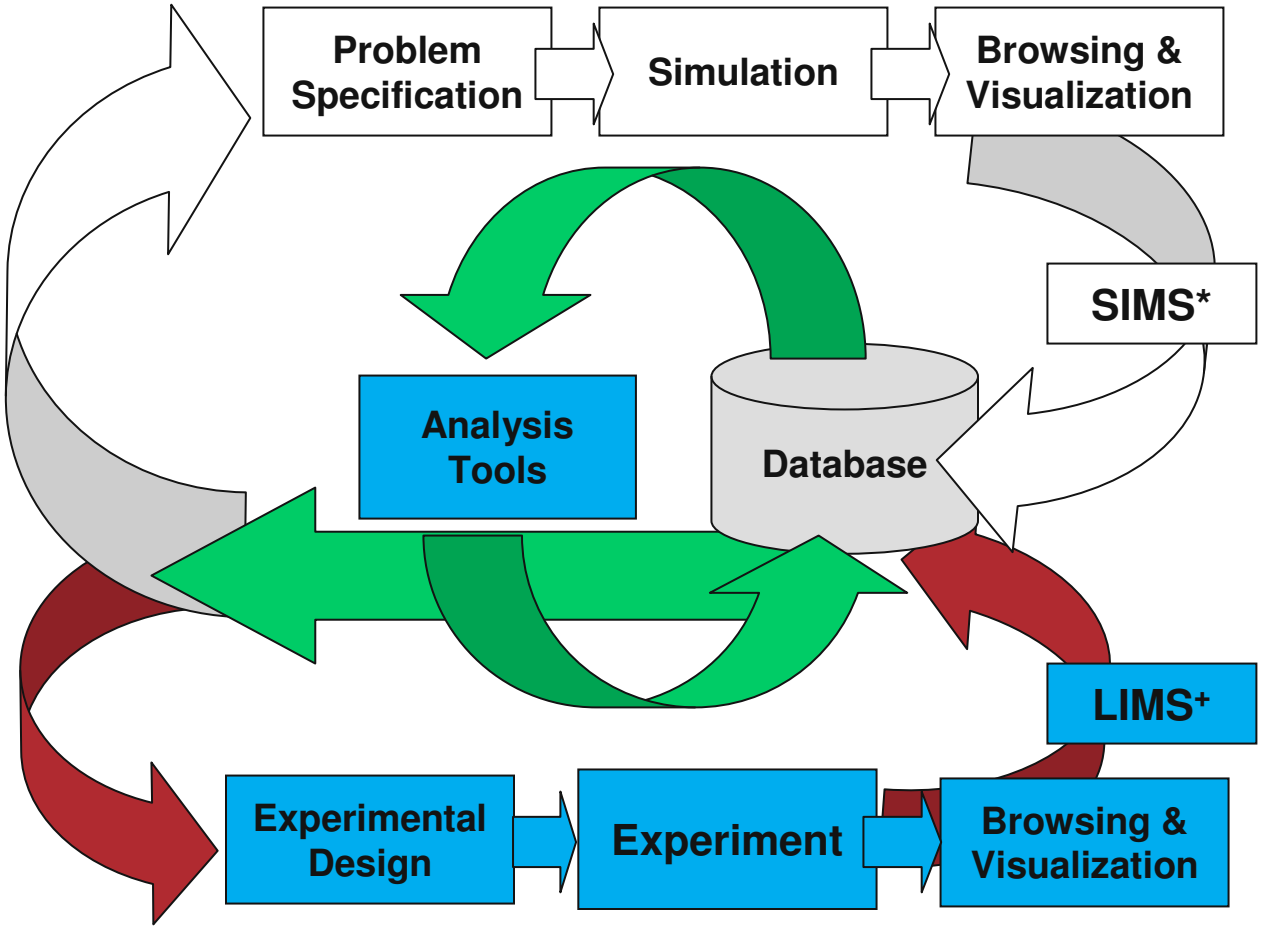
Common Characteristics

- Long-term project to tackle a complex problem
- Construction of sophisticated modeling systems
- Component-based to facilitate experimentation
- Work performed by a multidisciplinary team
- An inordinate focus on validation
- Designed to use high-performance computing
- Provided to the community as a resource
- Used for many purposes
- Advances the field substantially

Future Directions

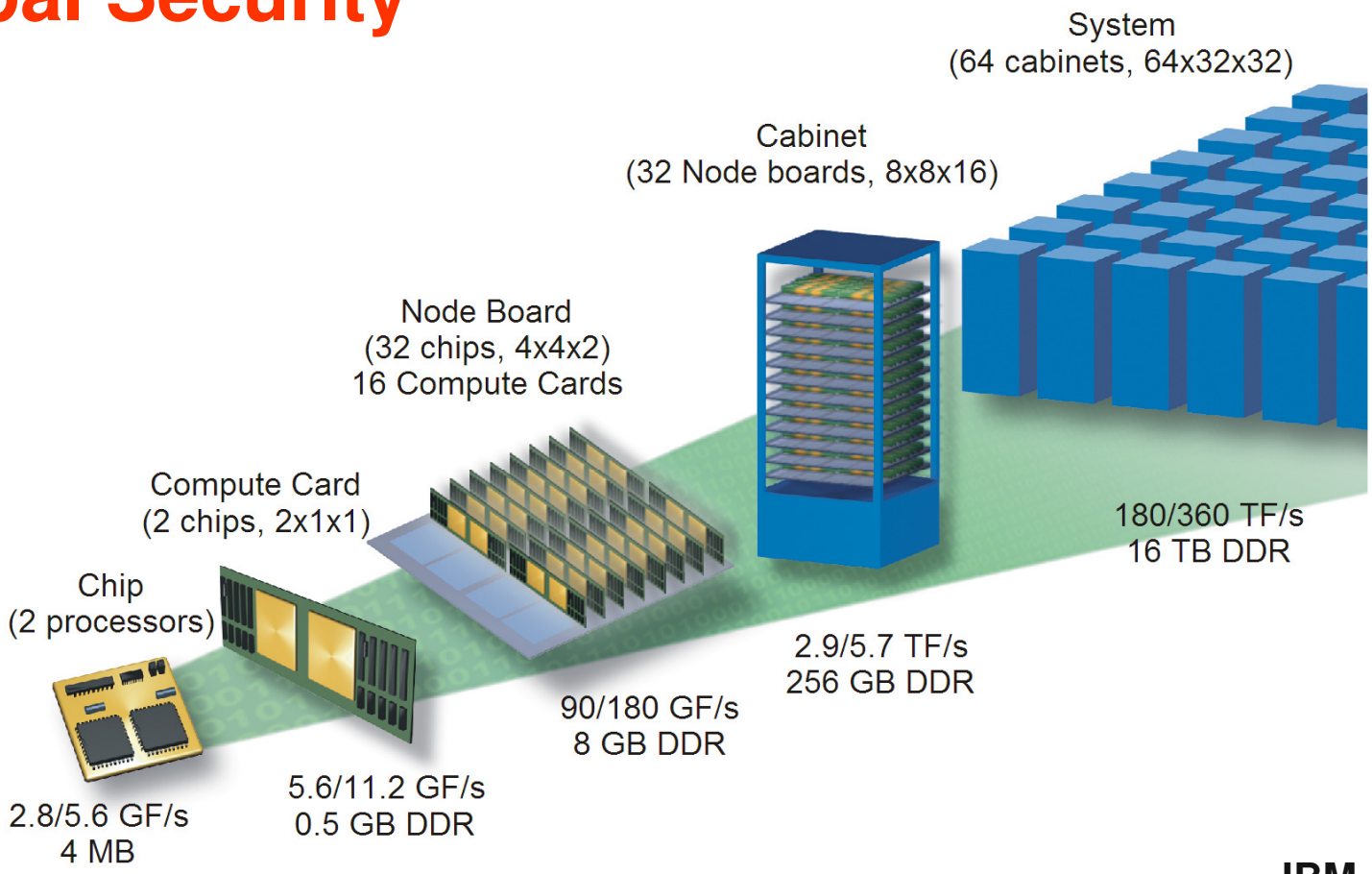
- Sensitivity analysis
  - E.g., automated development of adjoint models
- Data-intensive science—driven by “data big bang”
  - Peer-to-peer analysis and data product publishing
  - Distributed systems for automated analysis, discovery, and annotation
  - Automated hypothesis creation tools for pattern detection—capable of suggesting relationships
  - Predictive modeling

Beyond Models: An Integrated View of Simulation, Experiment, & (Bio)informatics



*Simulation Information Management System
+Laboratory Information Management System

Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security



IBM

Socio-Economic Modeling

Terascale (i.e., today, almost)

- Economic models with ~10 countries & ~10 sectors
- Limited coupling with climate models
- No treatment of uncertainty and business cycle risk
- Simple impact analysis for a limited set of scenarios
- Limited ability to provide quantitative policy advice

Socio-Economic Modeling

Petascale

- Economic models with more countries, sectors, income groups
- Limited treatment of uncertainty, business cycle risk
- Stronger coupling with climate models

Socio-Economic Modeling

Exascale

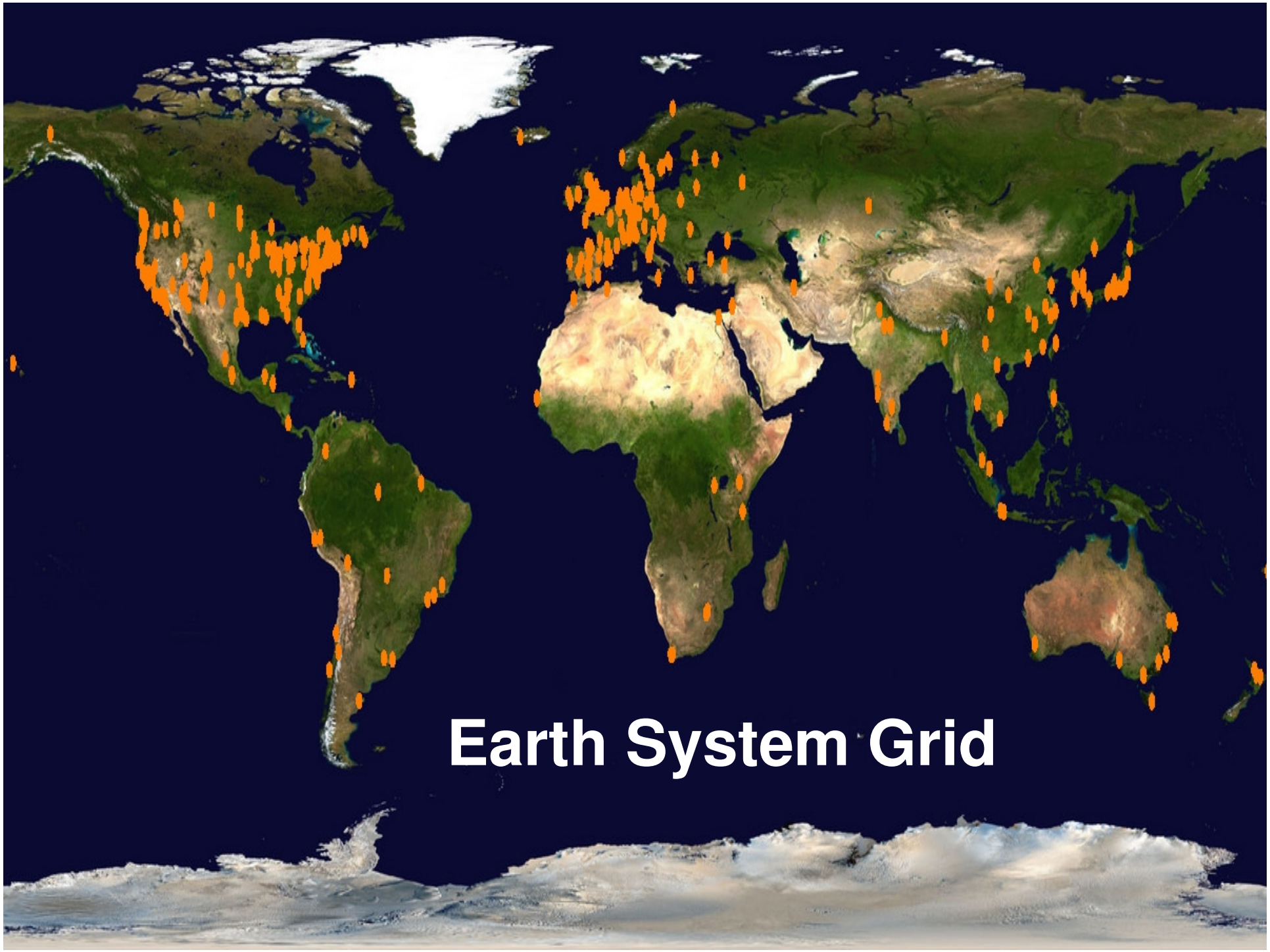
- Economic models with all countries, many sectors, many income groups
- Many policy instruments (taxes, tariffs, quotas, CAFE, CO2 taxes), nonlinear policies, etc.
- High spatial resolution in land use, etc.
- Detailed coupling & feedbacks with climate models
- Optimization of policy instruments & technology choices over time and with respect to uncertainty
- Detailed model validation & careful data analysis
- Treatment of technological innovation, industrial competition, population changes, migration, etc.

Pet

Tera

Meta-Innovation: How Can We Accelerate Innovation?

- We have discussed the usual ideas
  - Policies to encourage private R&D investment
  - Government investment in R&D
  - Education
- Can we use technology to accelerate innovation?
  - Lack of innovators: engage the world (Wikipedia)
  - Access to information: a “US Knowledge Exchange”
  - Access to modeling: models, tools, supercomputers


Earth System Grid

Meta-Innovation: How Can We Accelerate Innovation?

- We have discussed the usual ideas
  - Policies to encourage private R&D investment
  - Government investment in R&D
  - Education
- Can we use technology to accelerate innovation?
  - Lack of innovators: engage the world (Wikipedia)
  - Access to information: a “US Knowledge Exchange”
  - Access to modeling: models, tools, computers

Meta-Innovation: How Can We Accelerate Innovation?

- We have discussed the usual ideas
  - Policies to encourage private R&D investment
  - Government investment in R&D
  - Education
- Can we use technology to accelerate innovation?
  - Lack of innovators: engage the world (Wikipedia)
  - Access to information: a “US Knowledge Exchange”
  - Access to modeling: models, tools, supercomputers
- How to represent technology-accelerated innovation?