DEPARTMENT OF
SUSTAINABLE DEVELOPMENT

International Conference on:
„Implementation of the UN 2030 SDGs in the Black Sea Region"

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Multiscale & Multiphysics Modelling & Simulation Concepts for Addressing Sustainability

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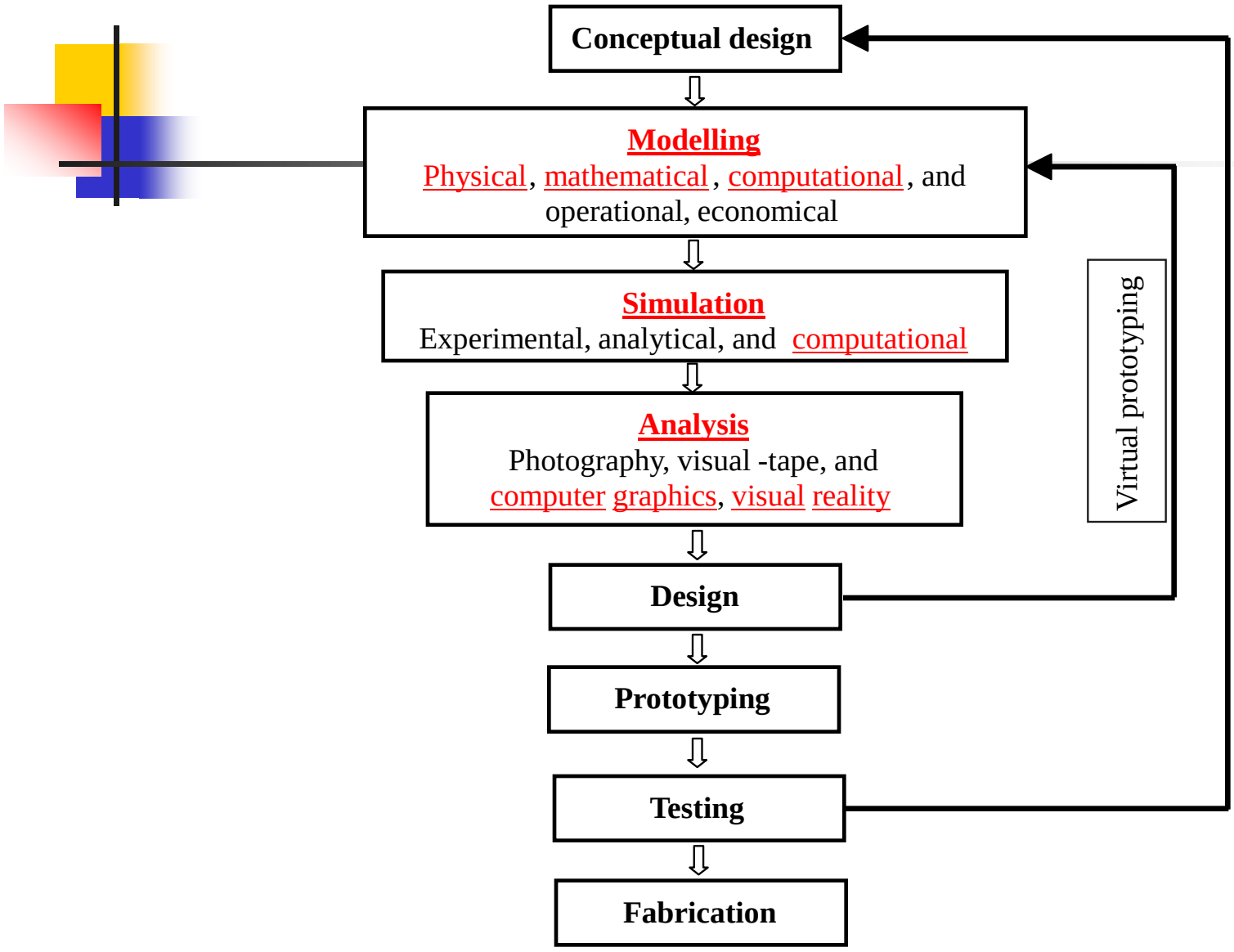
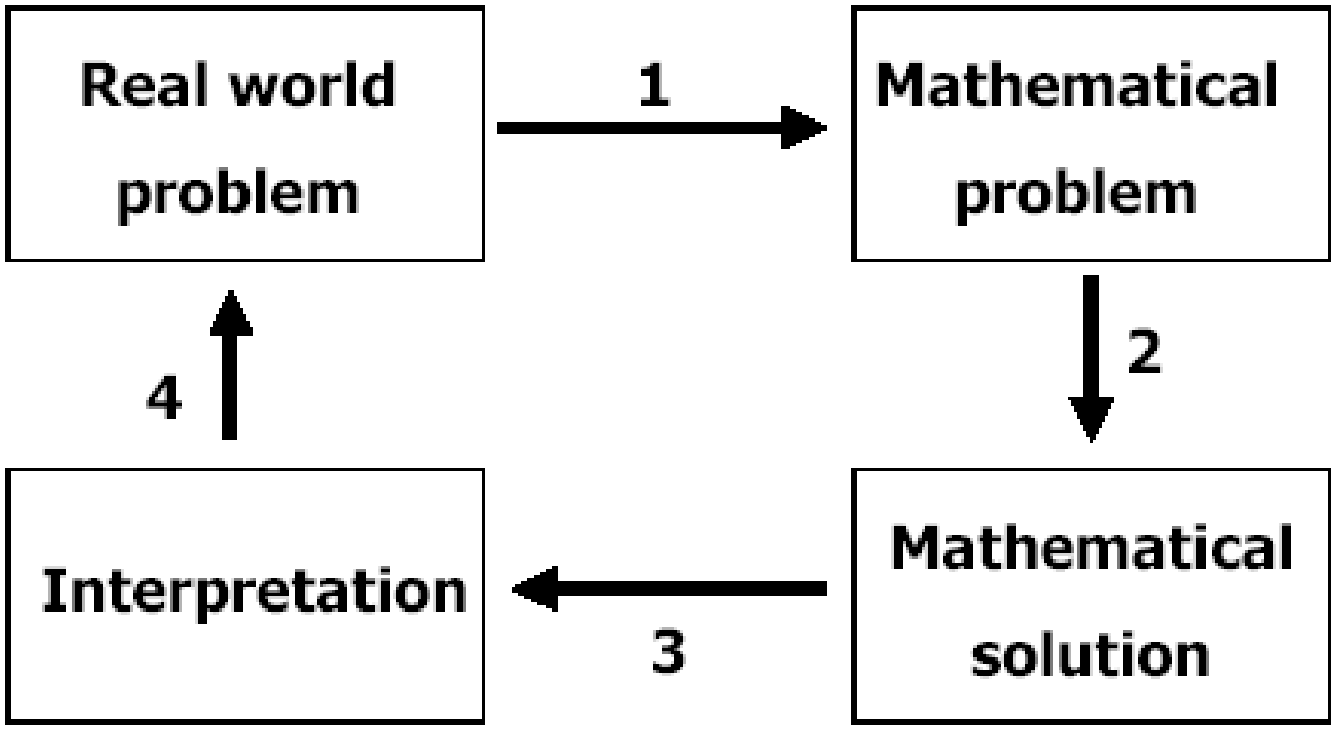
Black Sea Universities Network

OUTLINE

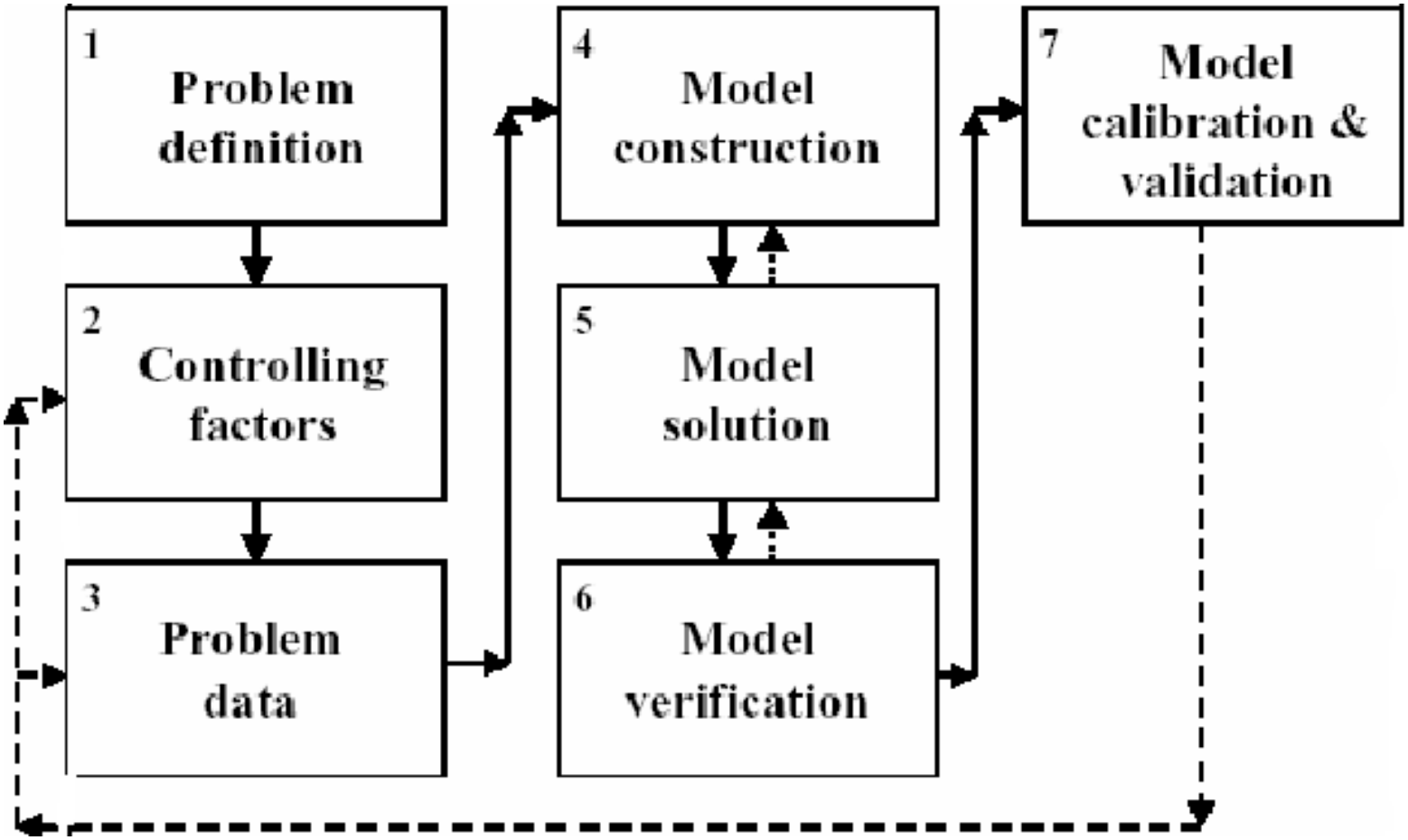
1. Modelling and simulation in engineering
2. Complexity of ecosystems
3. Multi-scale & Multi-physics
4. Available tools
5. Conclusions


Conceptual design
Modelling
Physical, mathematical, computational, and operational, economical
Simulation
Experimental, analytical, and computational
Analysis
Photography, visual -tape, and computer graphics, visual reality
Design
Prototyping
Testing
Fabrication
Virtual prototyping

MODELING PROCESS



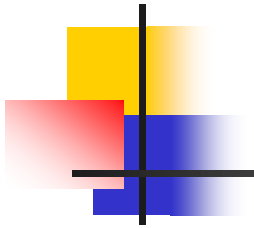
MODELING PROCEDURE



MODEL CONSTRUCTION

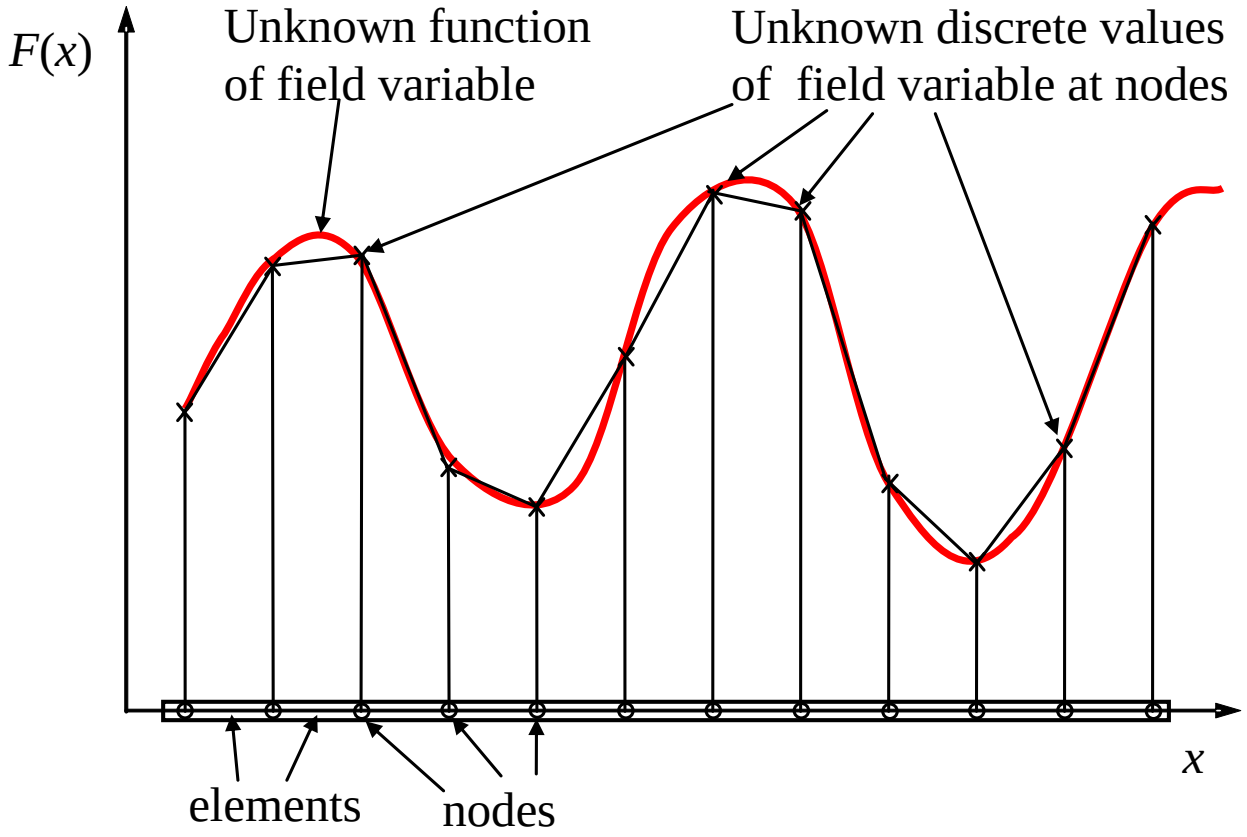
- Assumptions
- Boundaries and balance volumes
- Conservation equations
  - mass
  - energy
  - momentum
- Constitutive equations
  - reaction rates
  - transfer rates property relations
  - balance volume relations
  - control relations & equipment constraints
- Characterizing Variables
- Conditions (ICs, BCs)
- Parameters

MODEL SOLUTION

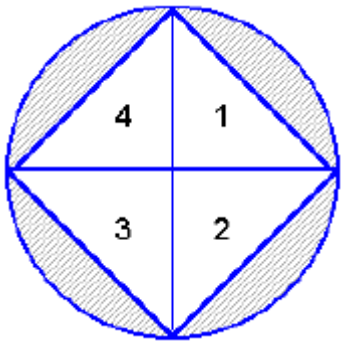


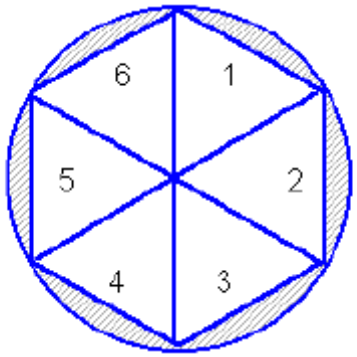
- Algebraic systems
- Ordinary differential equations
- Differential-algebraic equations
- Partial differential equations
- Integro-differential equations

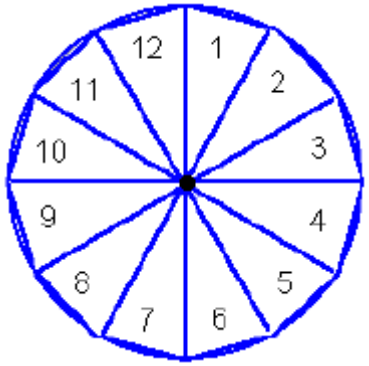
Discretization



Discretization

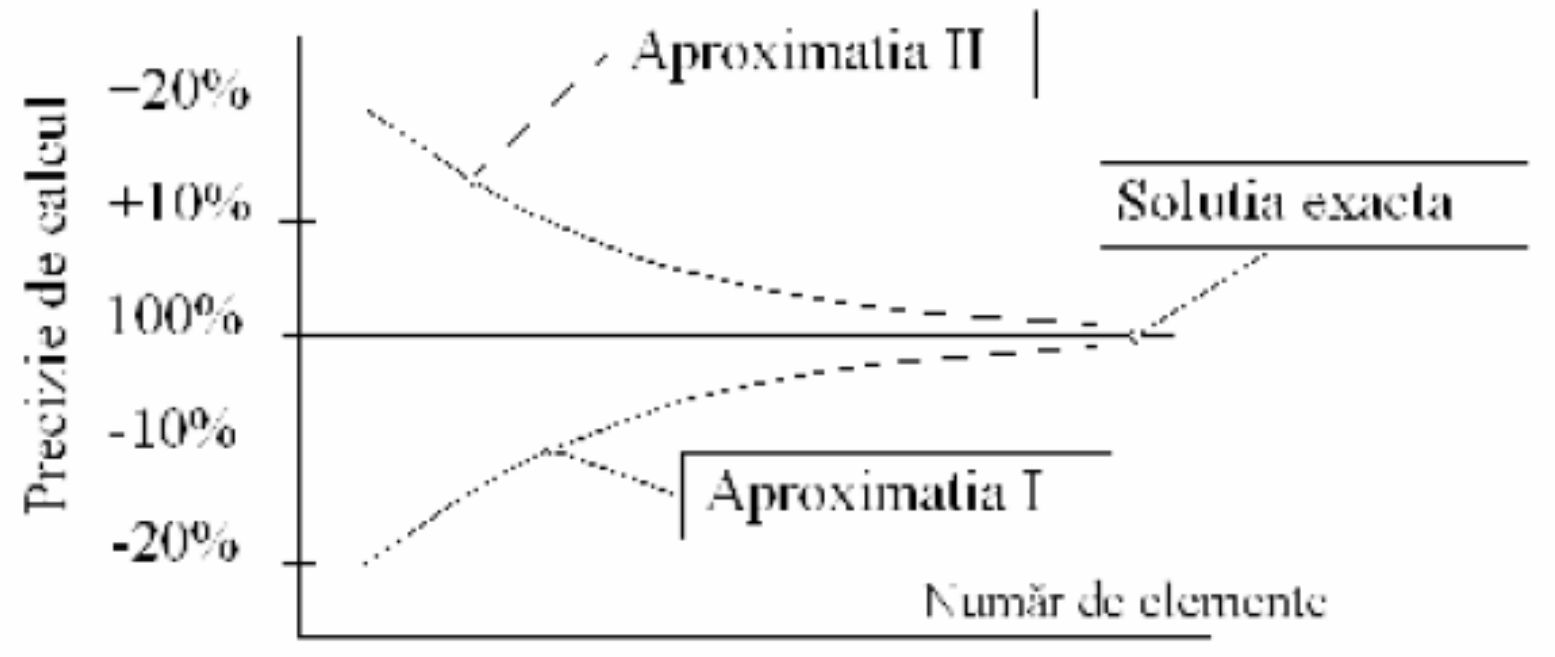






A_{tr} = b h/2 $\Longrightarrow$ Acerc = $\sum_{i=1}^{n} A_{tr\,i}$

Discretization



Computational volume 1

- **Typical example**: Solution of the laminar Navier – Stokes equations for viscous flow of an incompressible fluid, in velocity-vorticity form
- **2D**: **independent variables**: velocity vector $\underline{u}$ (u, v), vorticity rot $\underline{u}$
  - **System of equations**: 3 nonlinear PDEs
  - **Method**: 4th order Finite Difference Method (FDM)
  - **Mesh**: rectangular domain with 50 grid lines in each space direction
  - **Unknowns**: 50 x 50 x 3 = 7500
  - **Nonzero elements**: 50 x 50 x 9 (elements) x 9 (diagonals) = 203 000
  - **Full matrix**: $7500^2 = 56.3 \times 10^6$
- **3D**: **independent variables**: velocity $\underline{u}$ (u, v, w), vorticity rot $\underline{u}$
  - **System of equations**: 6 nonlinear PDEs
  - **Unknowns**: 50 x 50 x 50 x 6 = 750 000
  - **Nonzero elements**: 50 x 50 x 50 x 36 x 13 = 58.5×10^6
  - **Full matrix**: $750\,000^2 = 563 \times 10^9$

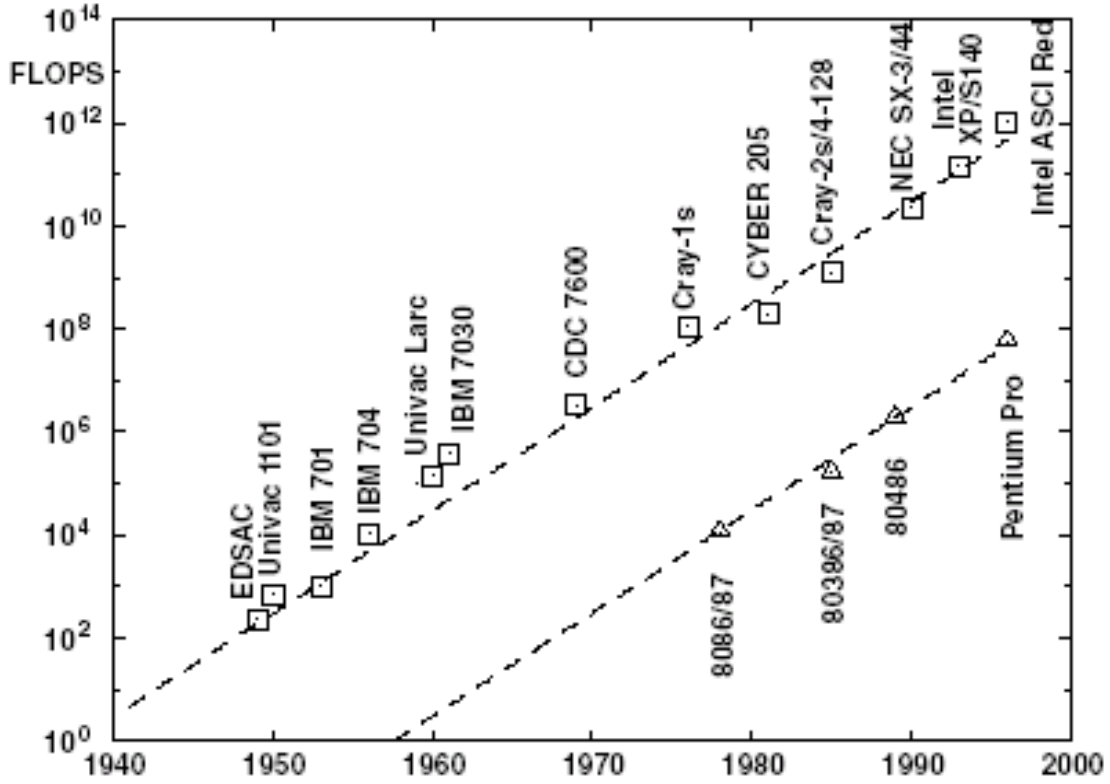
Computational volume 2

- **Flow around a structure**: 500^3 grid, 750×10^6 unknowns, 58.5×10^9 nze

- **Types of computers**:
  - SISD – Single Instruction stream / Single Data stream
  - SIMD – Single Instruction stream / Multiple Data stream
  - MIMD – Multiple Instruction stream / Multiple Data stream

- **Computer performances**:
  - Shared memory vector computer: $r_{sustained} = 0.1\ r_{theoret}$
  - Massively parallel computer: $r_{sustained} = 0.01\ r_{theoret}$

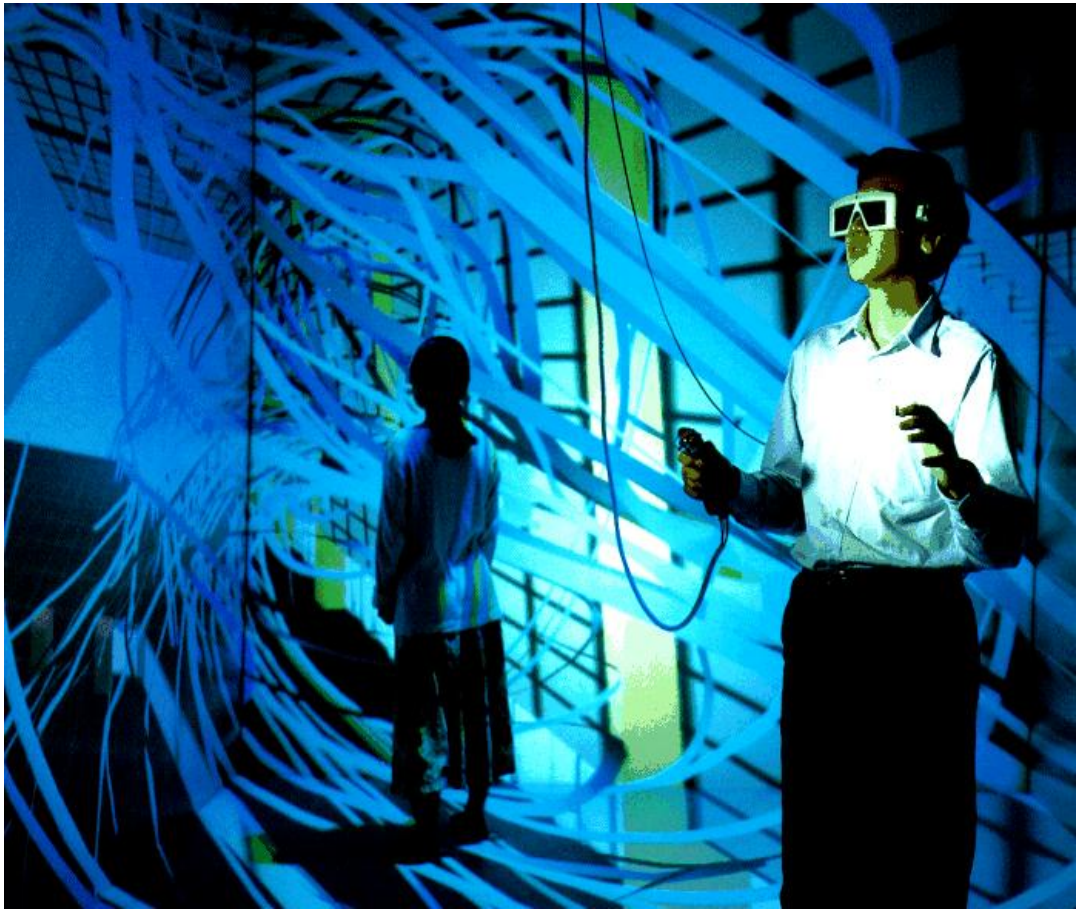
Evolution of processing power



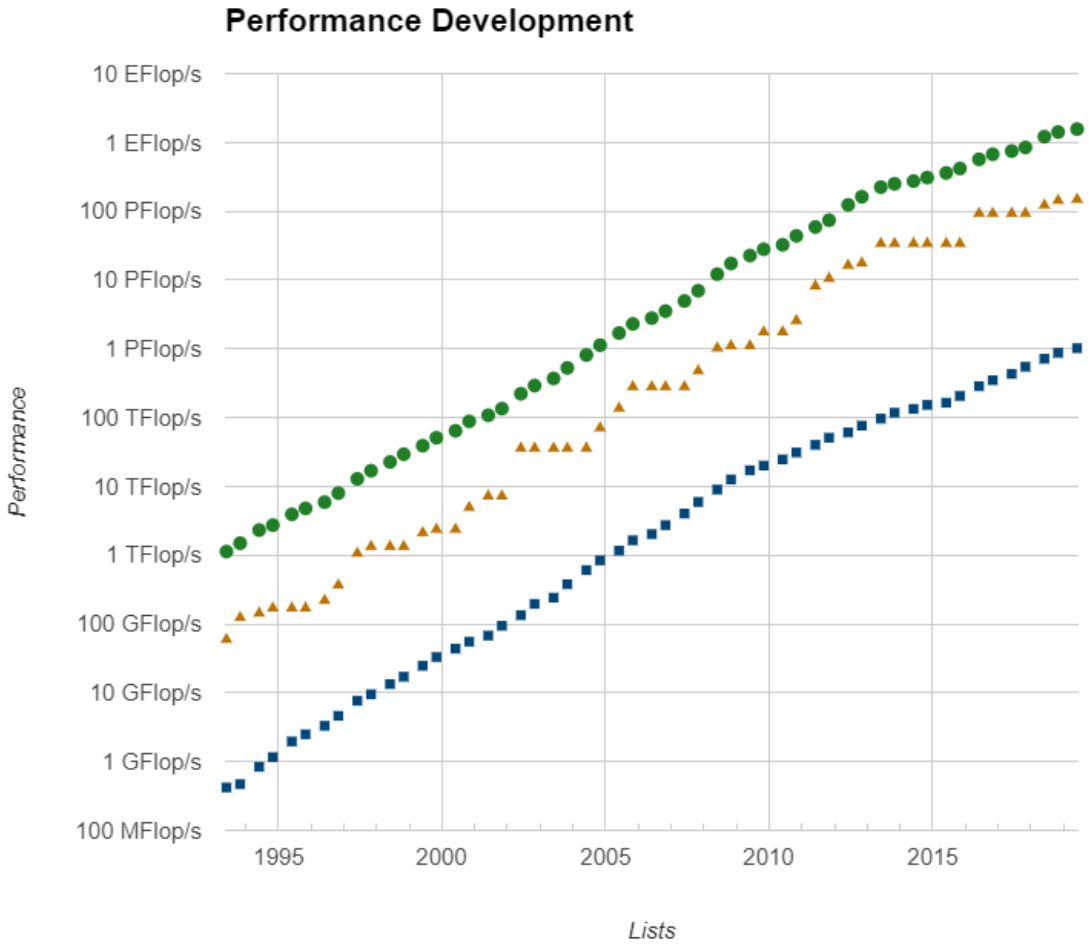
Peak performance development for supercomputers & PC processors

(Bartels, C. et al. 2002)

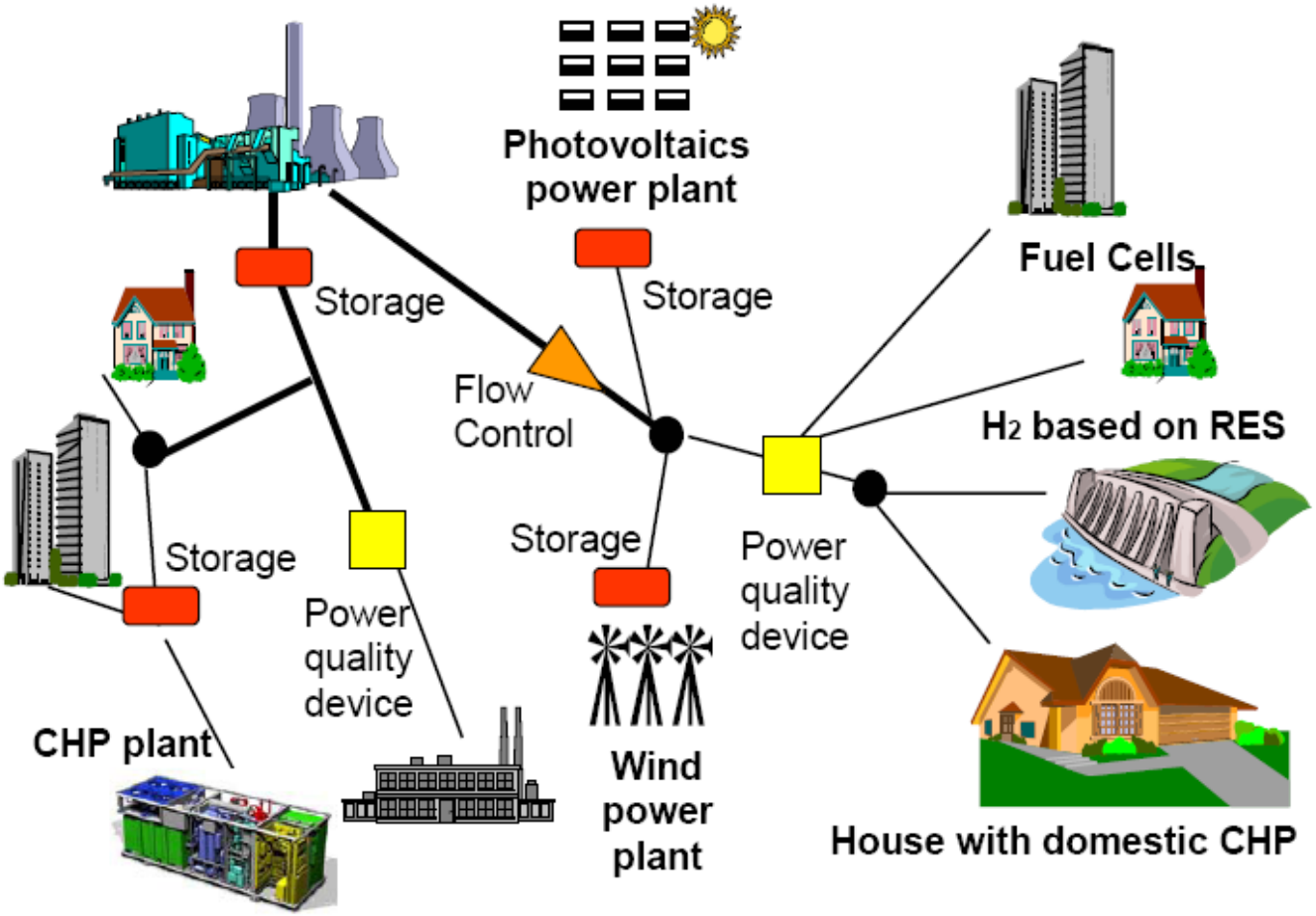
Simulation



Supercomputers

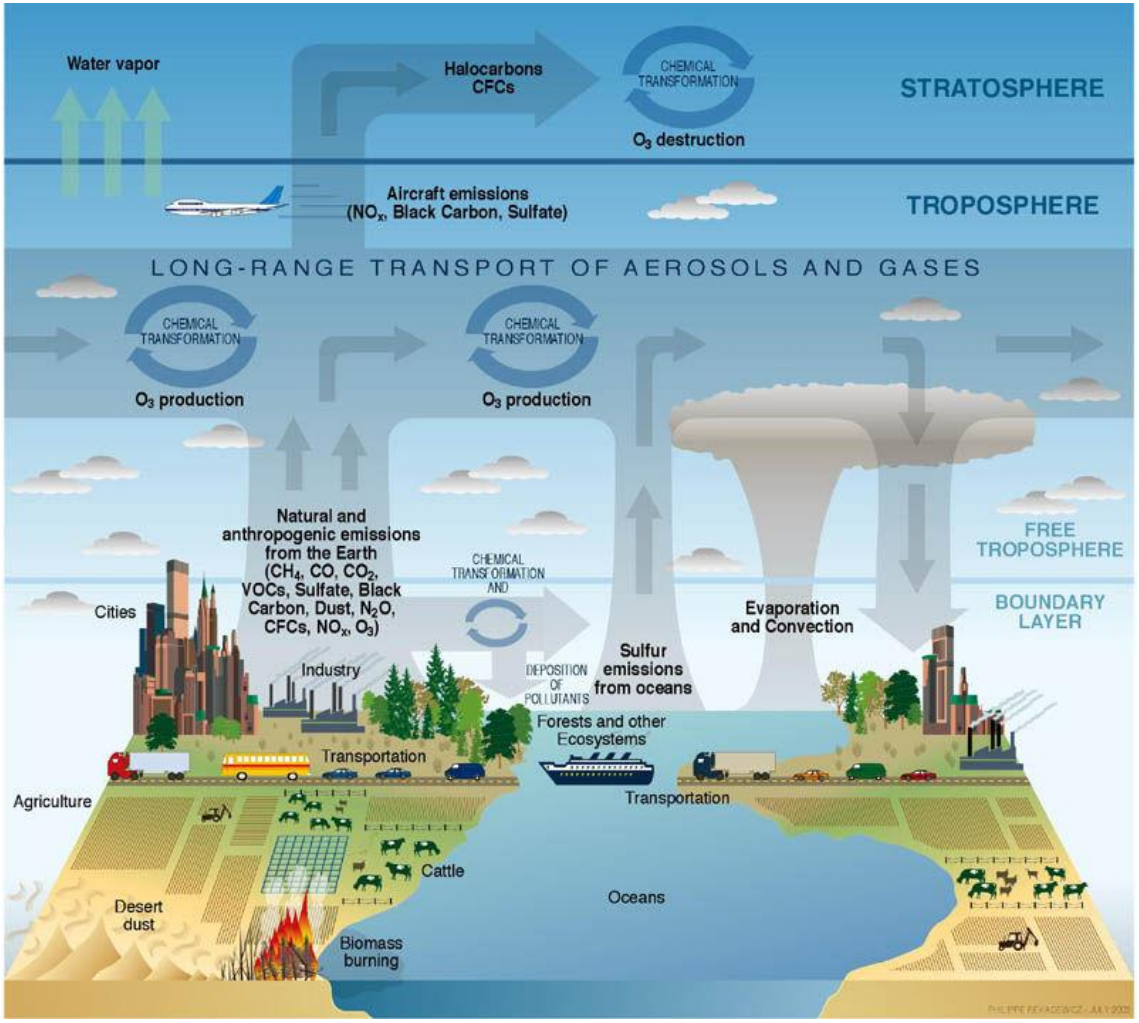


DISTRIBUTED ENERGY RESOURCES

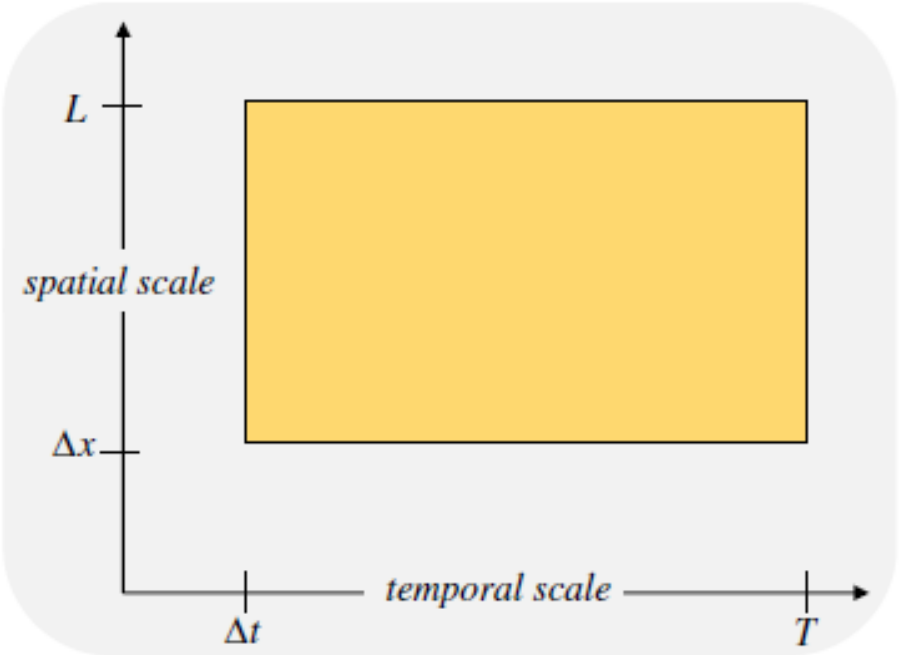


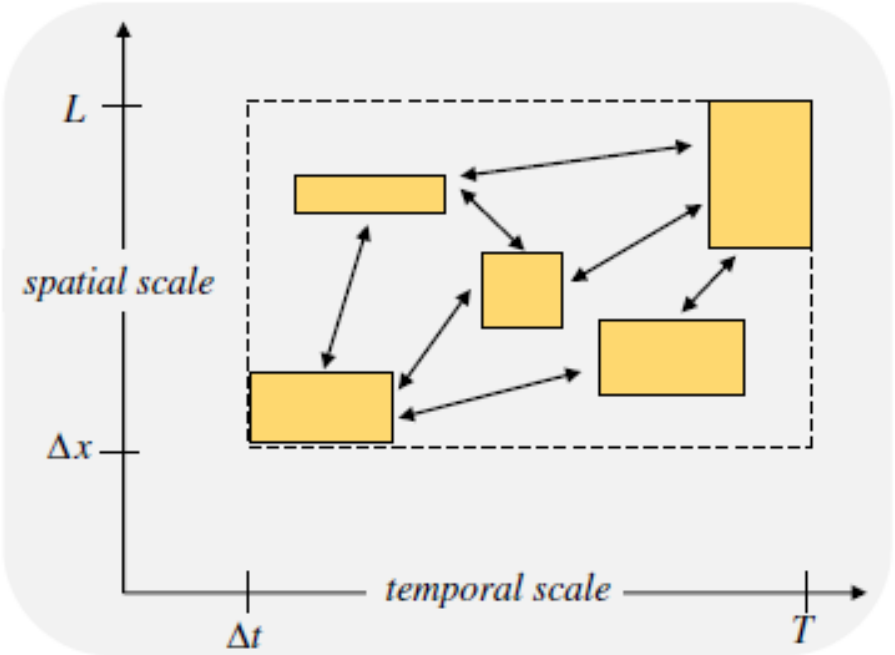
SOLAR ENERGY PLATFORM

Ecosystems


Water vapor
Halocarbons CFCs
CHEMICAL TRANSFORMATION
O_3 destruction
STRATOSPHERE
Aircraft emissions (NO_x, Black Carbon, Sulfate)
TROPOSPHERE
LONG-RANGE TRANSPORT OF AEROSOLS AND GASES
CHEMICAL TRANSFORMATION
O_3 production
CHEMICAL TRANSFORMATION
O_3 production
Natural and anthropogenic emissions from the Earth (CH_4, CO, CO_2, VOCs, Sulfate, Black Carbon, Dust, N_2O, CFCs, NO_x, O_3)
CHEMICAL TRANSFORMATION AND
FREE TROPOSPHERE
BOUNDARY LAYER
Cities
Industry
DEPOSITION OF POLLUTANTS
Sulfur emissions from oceans
Evaporation and Convection
Forests and other Ecosystems
Transportation
Transportation
Agriculture
Cattle
Oceans
Desert dust
Biomass burning

Decomposition





DIMENSIONS & SCALES

Multidimensions:

- Economical;
- Ecological;
- Social & Institutional.

Multicriteria:

- Economical: Growth competitiveness index, Economic freedom index;
- Ecological: Environmental sustainability index;
- Social & Institutional: Quality of life index, Human development index, Knowledge society index.

DIMENSIONS & SCALES

Multiscales:

- System;
- Local cluster of end-users
- Urban / Rural agglomeration;
- Sub-region;
- Country;
- Region.

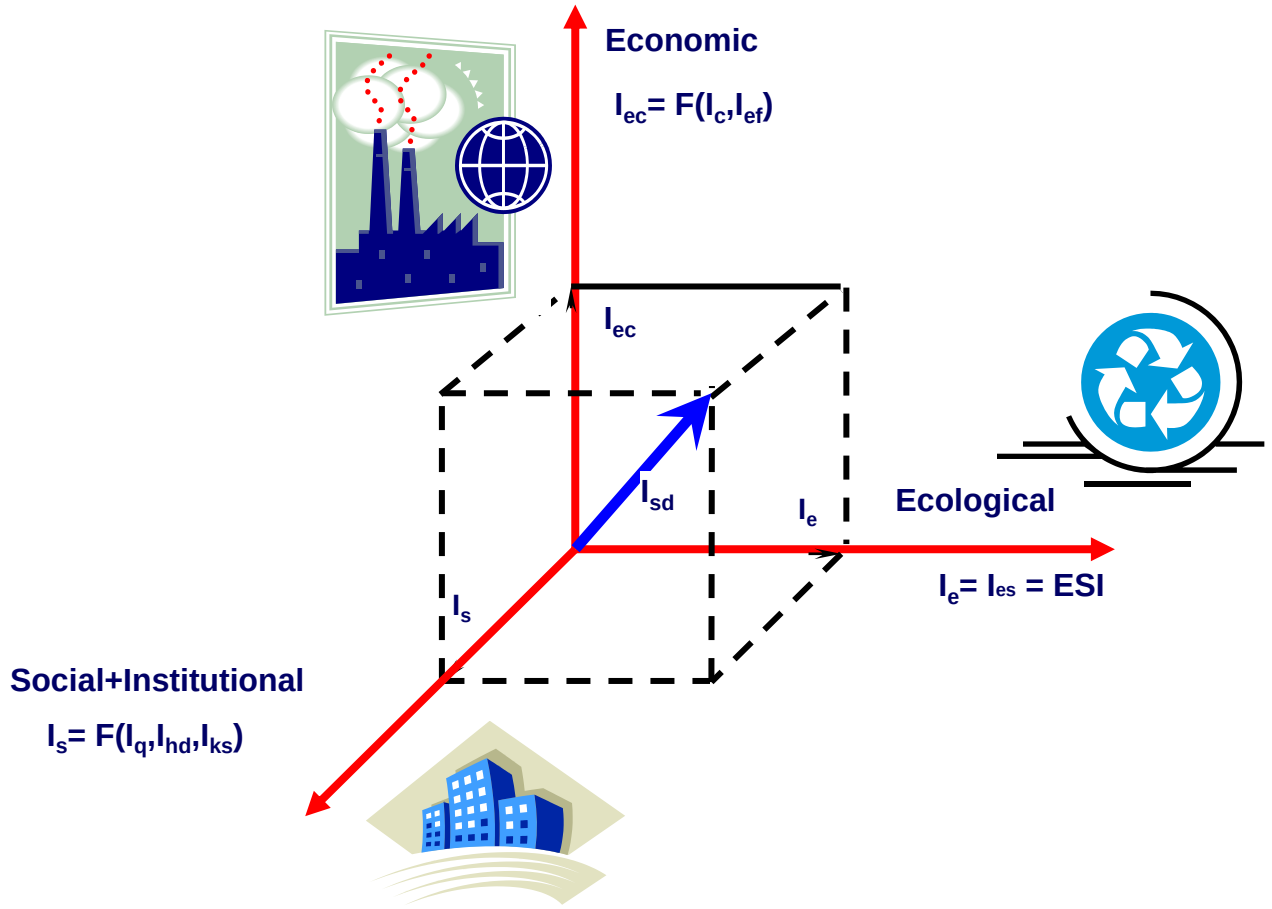
MULTI-DIMENSIONAL MODELING

Multi-dimensional models or „multi-scale" as well as the integrated multi-phenomenological models or „multi- physics" have been developed in time, covering today a large number of applications including the materials science, the nano/microelectronics, the ecological reconstruction, the deactivation of the atomic armament and biotechnologies.

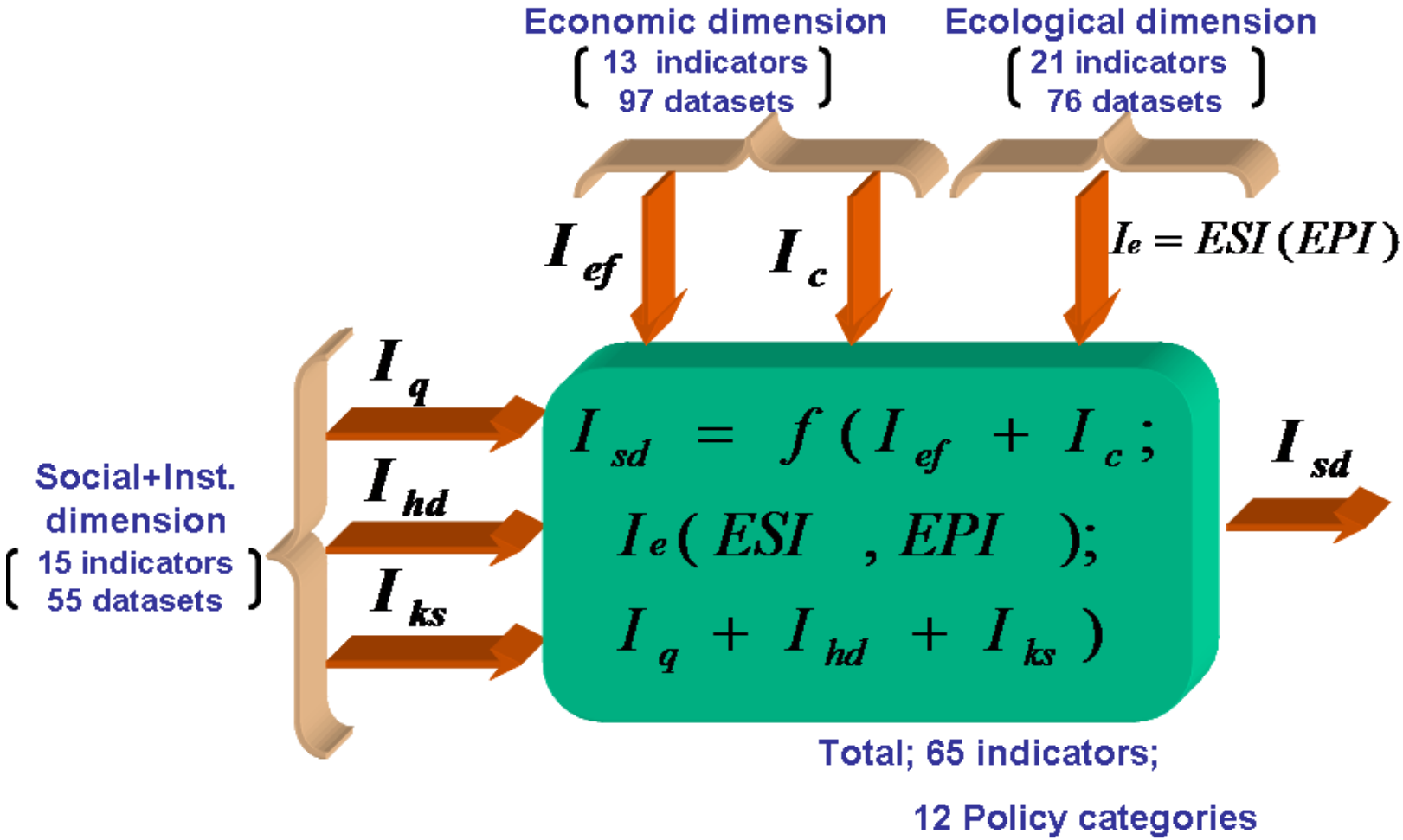
The multi-dimensional modeling approaches (MMD) can be grouped in the following generic categories:

- **MMD with the transfer of the parameters – which integrates two or more models associated to different dimensional and/or temporal scales and the resulted parameters based on a model are used as input data for the other models;**
- **MMD with simultaneously solved multi-dimensional models (in the way used in Concurrent Engineering) – which integrates more mutual influenced models which leads to the necessity of simultaneous simulations with mutual data exchange protocols;**
- **MMD unitary integrated – consisting of the use of a mathematical device that includes terms associated to different dimensional and/or temporal scales in a unitary configuration.**

GAUGING MATRIX OF SUSTAINABLE DEVELOPMENT



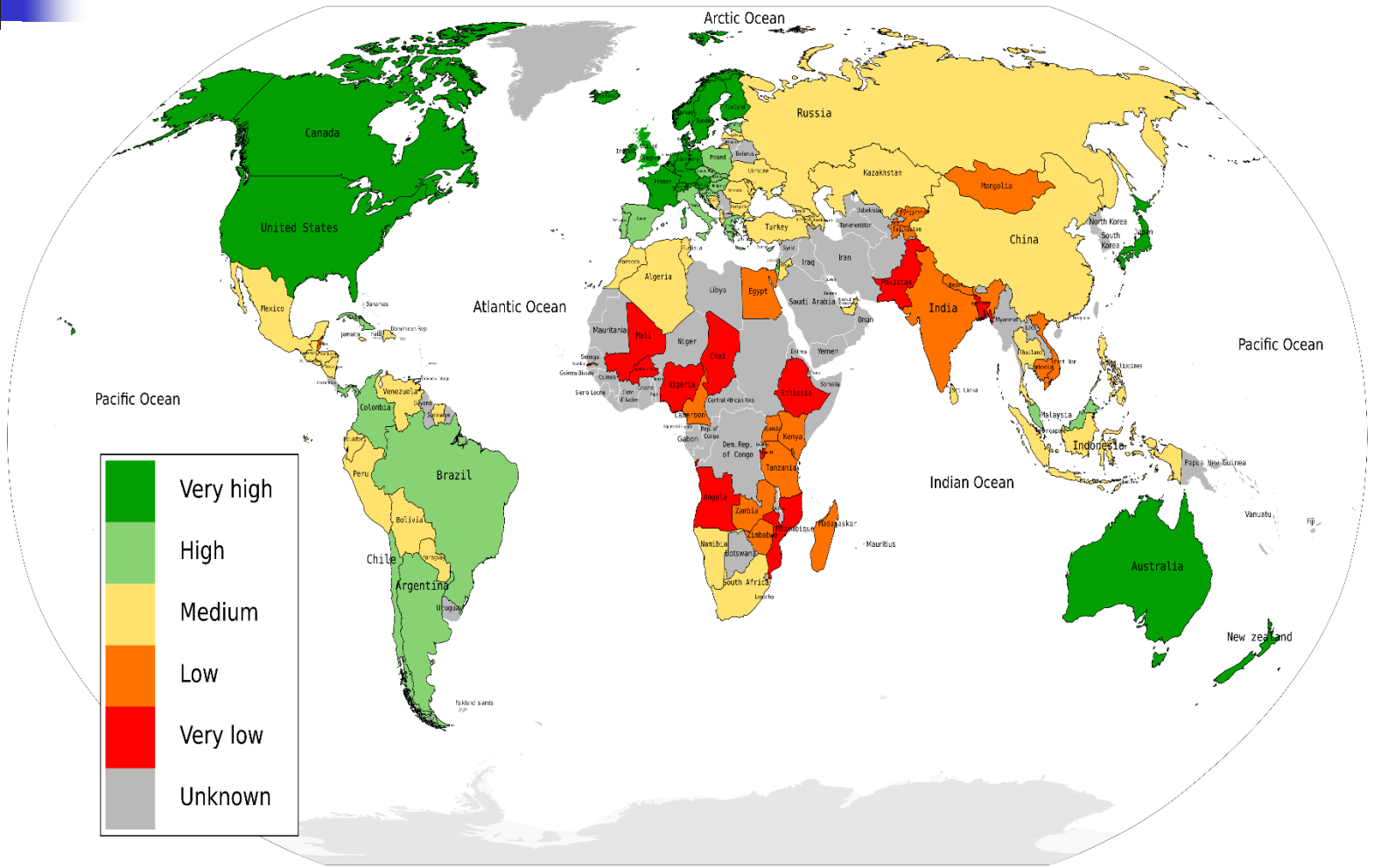
GENERAL MATHEMATICAL MODEL



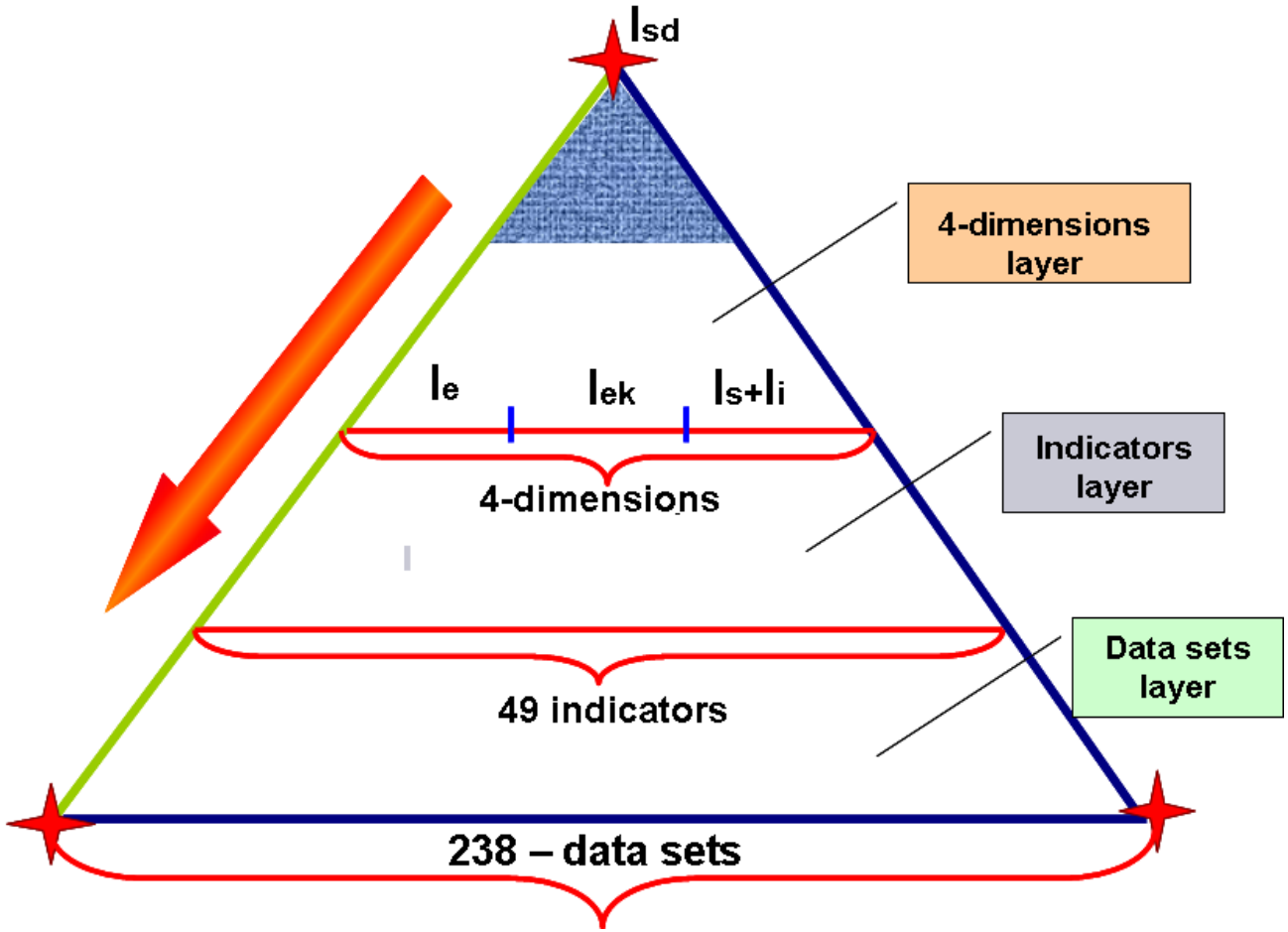
GLOBAL INDICES

Measure of sustainable development	Global Index	Constituents	Source
Economic (Iec)	Ic – Growth (Global) Competitiveness Index	3 indicators, 47 sets of data	World Economic Forum [www.weforum.org]
	Ief – Economic Freedom Index	10 indicators, 50 sets of data	Heritage Foundation [www.heritage.org]
Ecological (Ie)	Ies–Environmental Sustain-ability (Performance) Index	21 indicators, 76 sets of data	Yale University, USA [www.yale.edu/esi]
Social+ Institutional (Is)	Iq – Quality-of-Life Index	9 indicators	Economist Intelligence Unit [www.en.wikipedia.org]
	Ihd – Human Development Index	3 indicators 50 sets of data	United Nation Development program [www.hdr.undp.org]
	Iks – Knowledge Society Index	3 indicators, 15 sets of data	UNDESA,[UN publication, NE.04.C.1.2005]

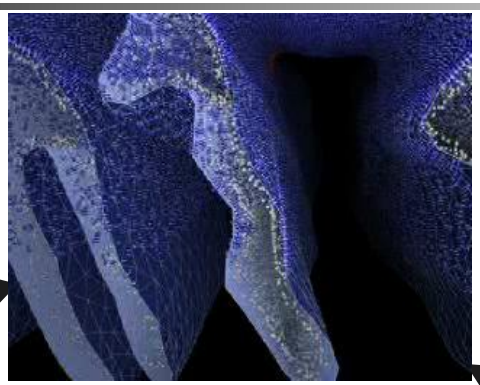
SUSTAINABLE DEVELOPMENT CLUSTER ANALYSIS



REVERSE ANALYSIS PROCEDURE



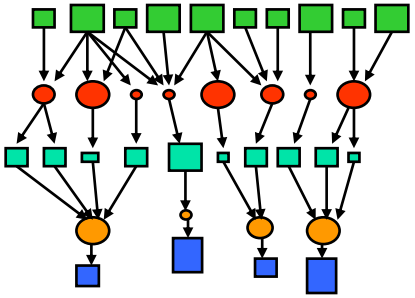
Complex applications



Models provide data for simulation

MCell as biologists see it

MCell as computer scientists see it



Shared Input data

Tasks

Raw Output

Post-processing

Final Output

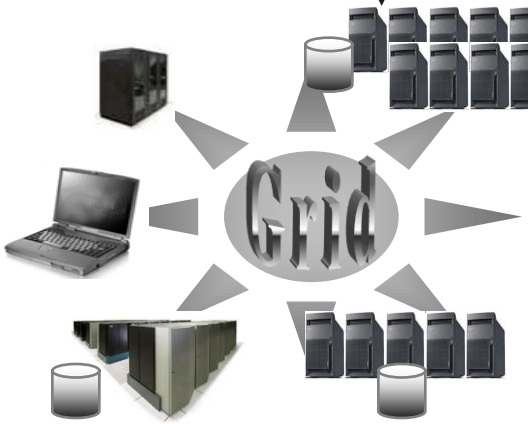
Simulation executed on available resources: supercomputers to lab clusters.

Feedback Improves model accuracy

Tomographic Reconstruction

Biological modeling from physical samples

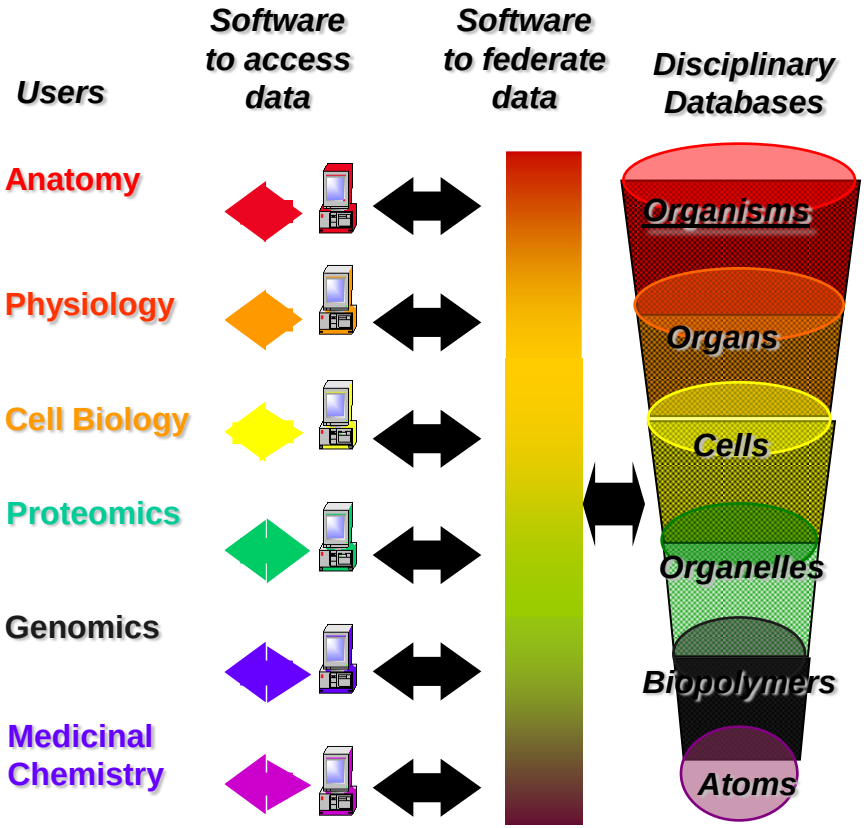
Electron Microscope



MCell code developed to target wide variety of technologies

Data Integration

Data Integration in the Biosciences

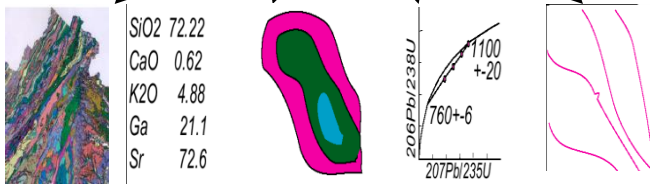


Data Integration in the Geosciences

Where can we most safely build a nuclear waste dump?
Where should we drill for oil?
What is the distribution and U/ Pb zircon ages of A-type plutons in a specific location?
How does it relate to host rock structures?

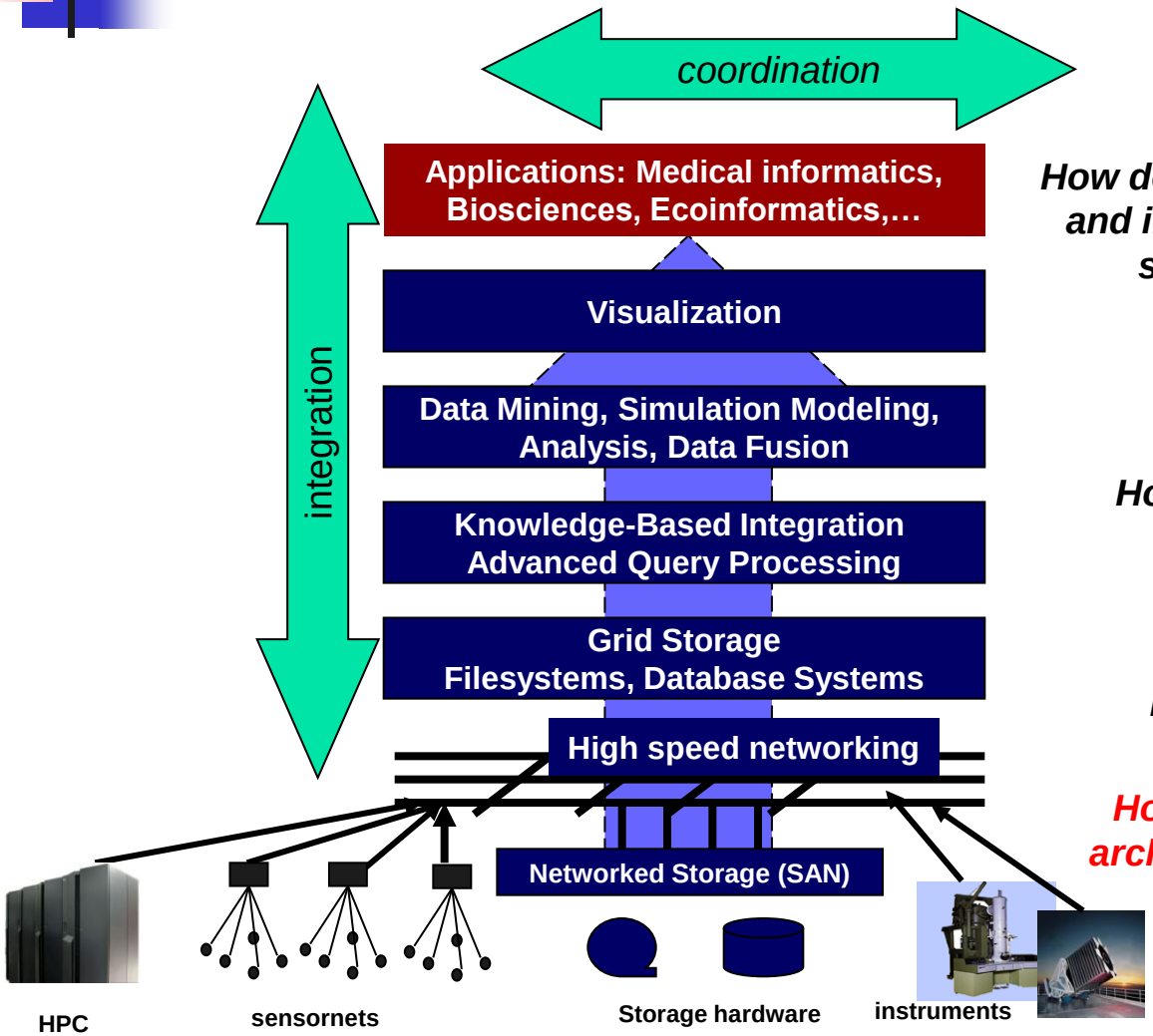
Data Integration

Complex "multiple-worlds" mediation



Geologic Map | *Geo-Chemical* | *Geo-Physical* | *Geo-Chronologic* | *Foliation Map*

Technical challenges



How do we combine data, knowledge and information management with simulation and modeling?

How do we represent data, information and knowledge to the user?

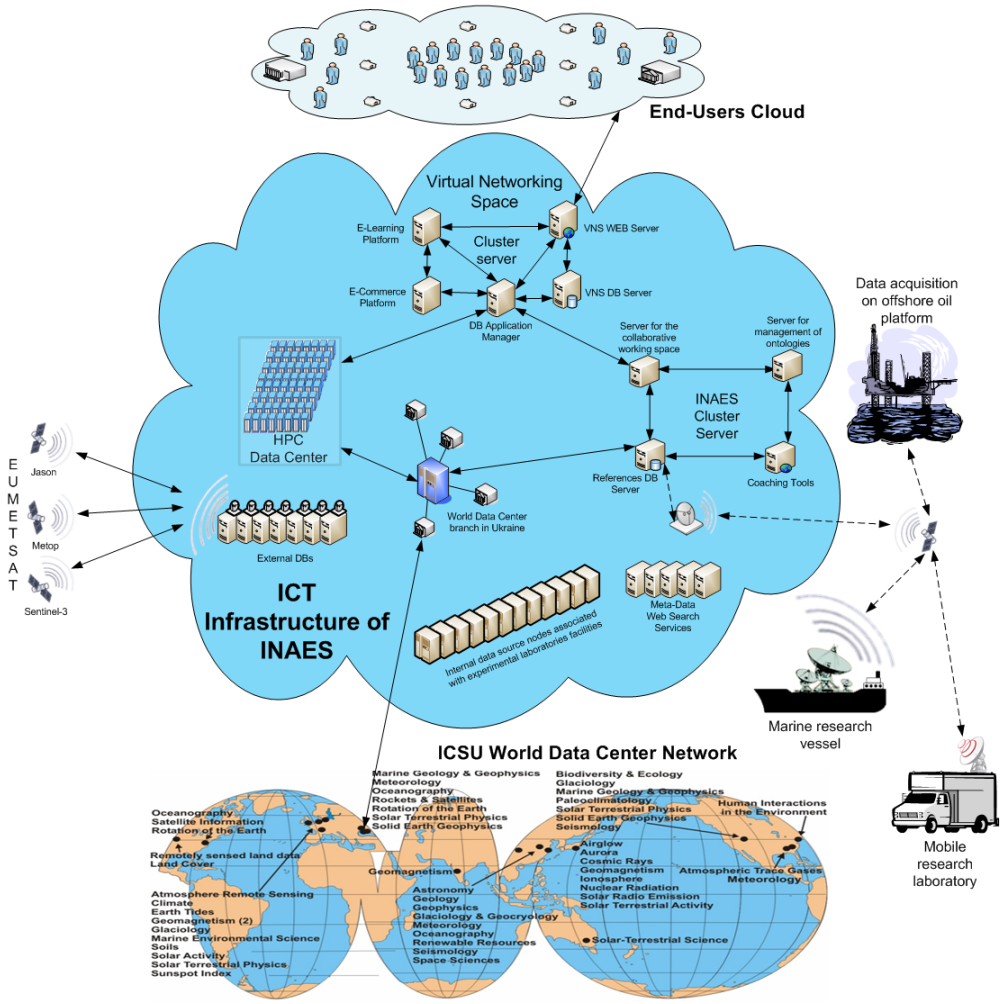
How do we detect trends and relationships in data?

How do we obtain usable information from data?

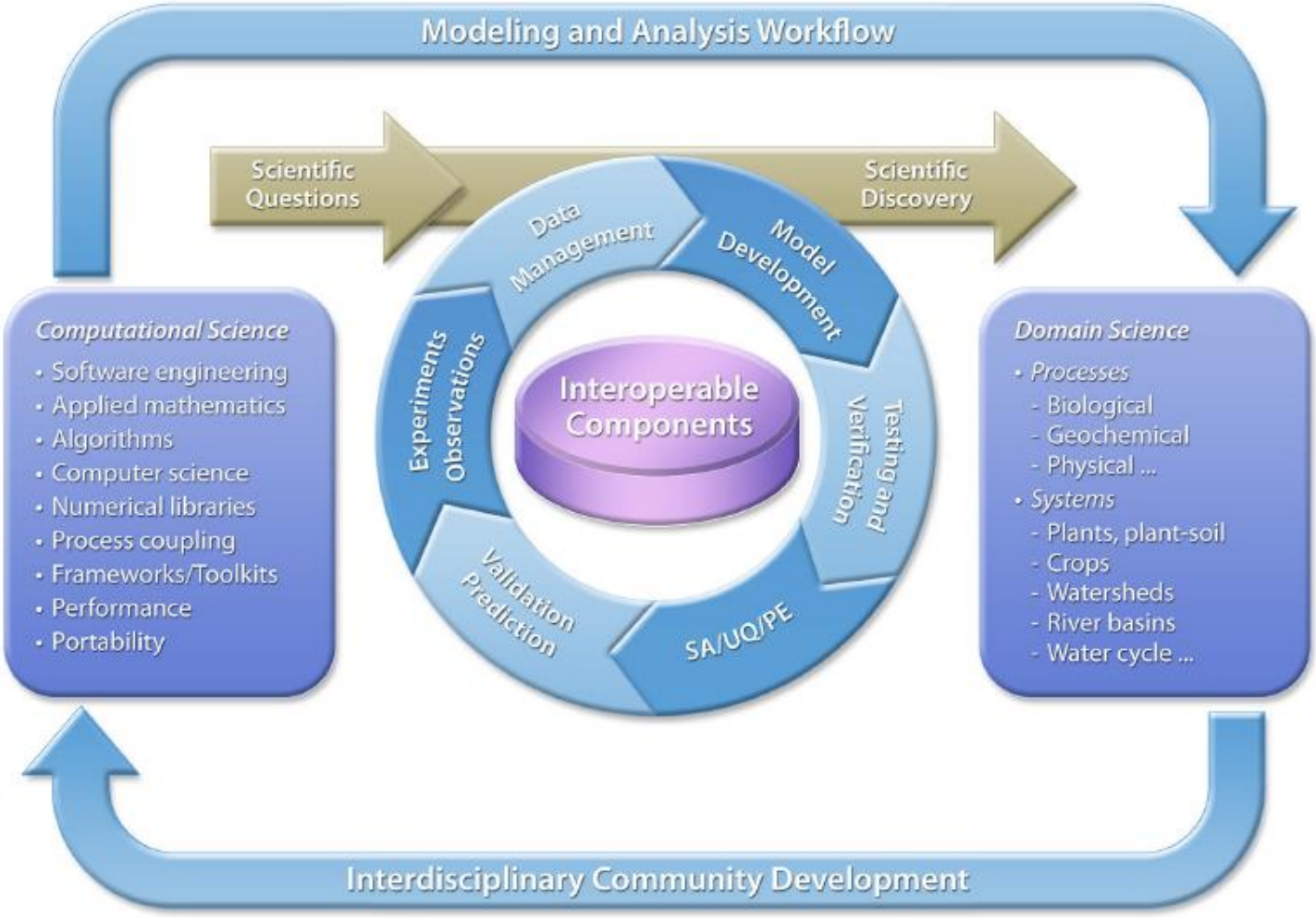
How do we collect, access and organize data?

How do we configure computer architectures to optimally support data-oriented computing?

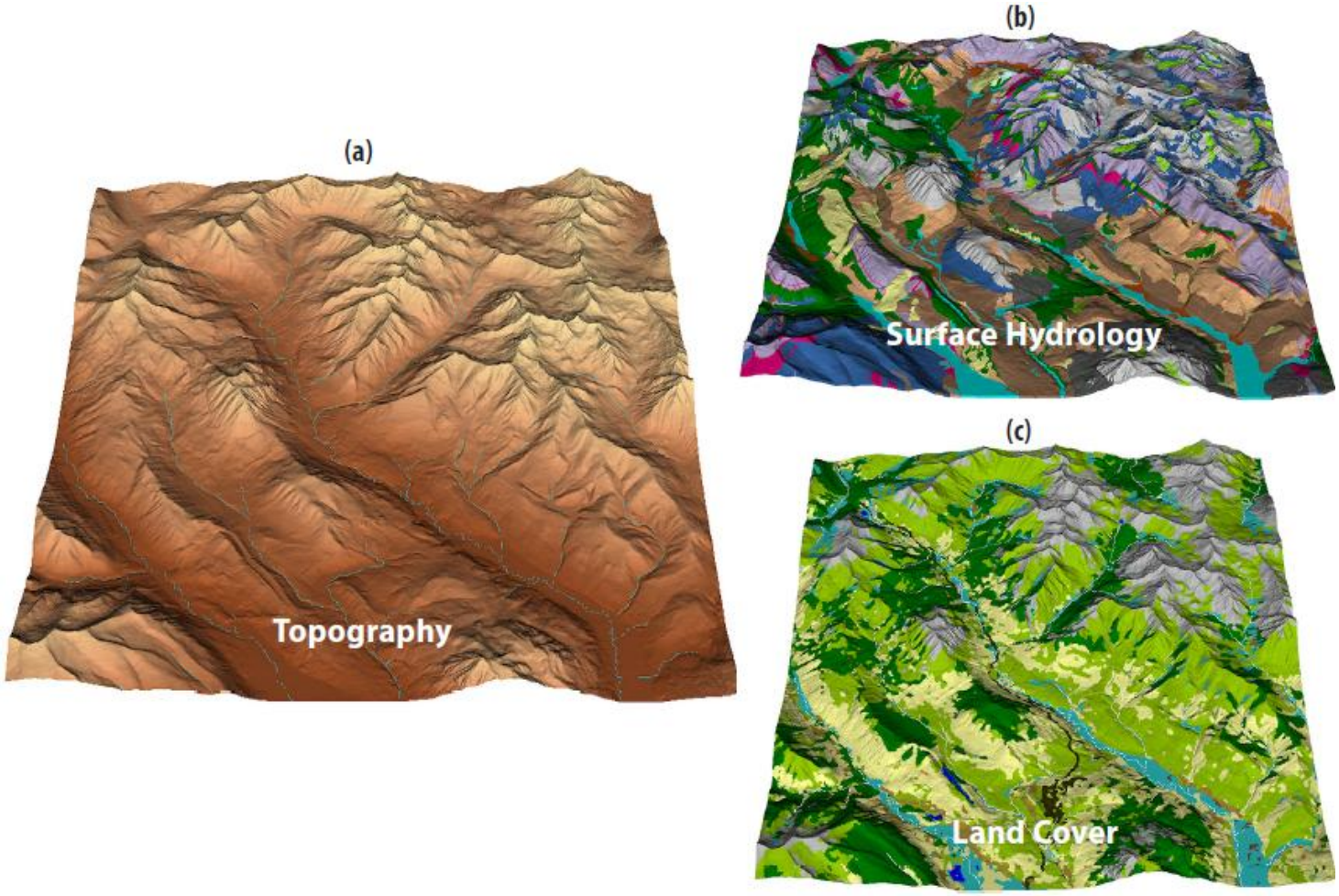
INTEGRATED PLATFORM



Modeling & Science



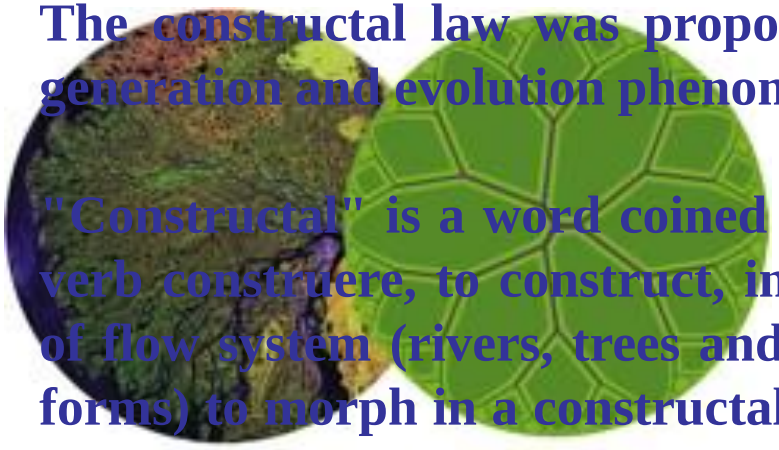
Modeling & Ecosystem Service



THE CONSTRUCTAL THEORY – ADRIAN BEJAN

"For a finite-size system to persist in time (to live), it must evolve in such a way that it provides easier access to the imposed currents that flow through it.“

Adrian Bejan, 1996



The constructal law was proposed in 1996 as a summary of all design generation and evolution phenomena in nature.

"Constructal" is a word coined by Adrian Bejan, coming from the Latin verb construere, to construct, in order to designate the natural tendency of flow system (rivers, trees and branches, lungs and also the engineered forms) to morph in a constructal evolutionary process toward greater and greater flow access in time.

Thank you for your attention!

and pleased, send your comments at:
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