"… The Wonderful becomes Familiar, and the Familiar fills you with Wonder…"

Stories from Process Systems Engineering by an Unindoctrinated Academic

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Massachusetts Institute of Technology
and
Arizona State University

25th Nordic Process Control Workshop
Aalto University, Espoo, Finland
February 15-17, 2025

Do not view Process Control in isolation.

It is part of the broader scope of
Process Systems Engineering

Period 1: University of Minnesota (1974-1985)

Questioning the Premises:
Recasting Old and Formulating New Problems

Period 2: MIT (1985-2000)

Becoming a student again: Computer science
Intelligent Systems for Process Engineering

Period 3: Mitsubishi Chemical Corporation (2000 – 2005)

The Most Fascinating Voyage of my Life

Period 4: MIT (2005 – 2015)

Becoming a student again: Statistical Mechanics and Control

Period 5: Reflections (2015 – now)

Putting everything together
Writing a book on "Chemical and Biological Process Dynamics and Control"

Period 1: University of Minnesota (1974-1985)

Questioning the Premises:
Recasting Old and Formulating New Problems

1. Interaction of Process Design and Control

2. Synthesis of Control Structures for Complete Chemical Plants

Interaction of Process Design and Control

Steady State Operability: Open and Closed

Dynamic Resilience

State or Input Steady State Multiplicity

Constraints and Steady State Optimal Operation

Synthesis of Control Structures for Complete Chemical Plants

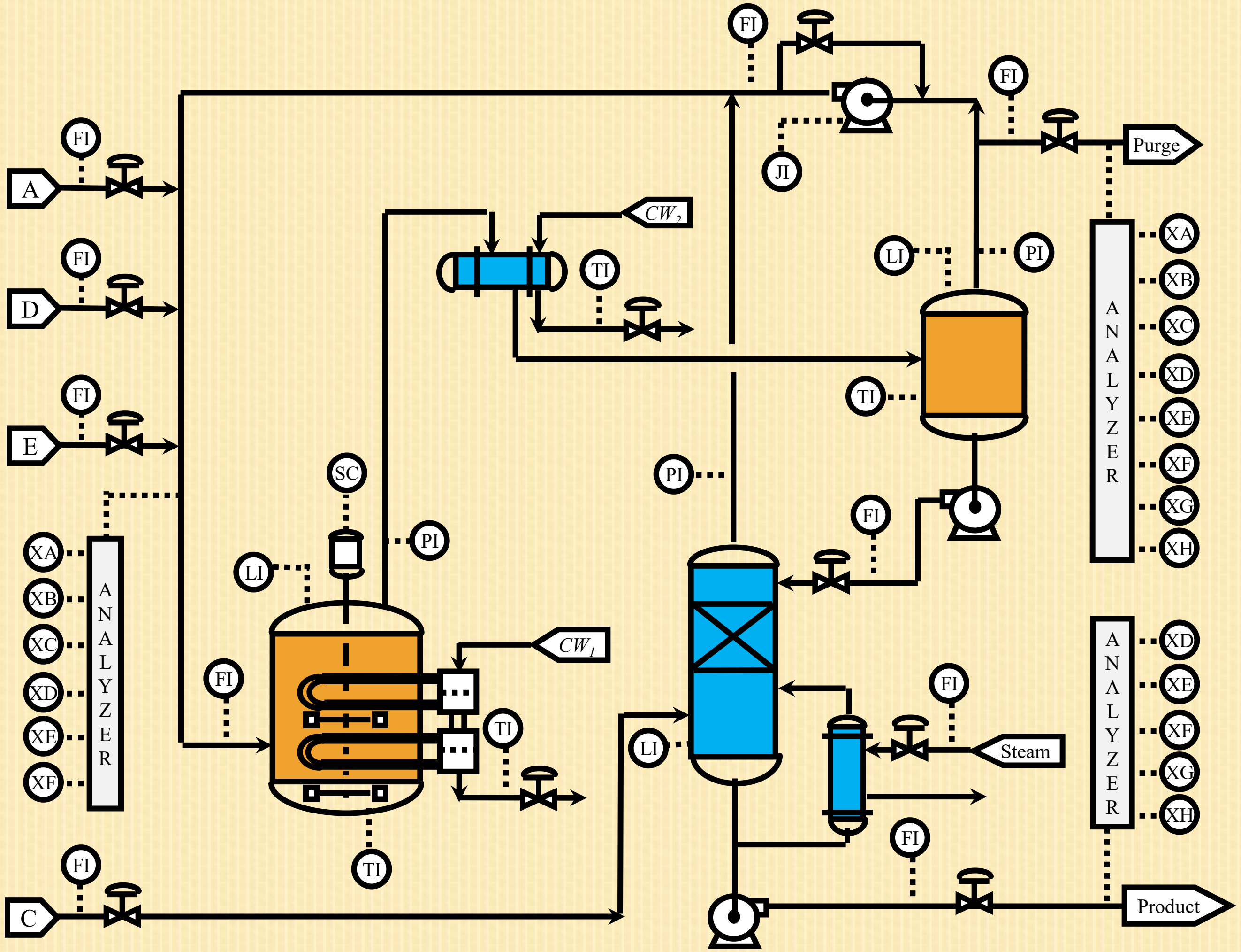
Perhaps the central issue to be resolved by the new theories of chemical process control is the determination of control system structure. Practicable solutions to this problem are not directly forthcoming from the current methods …The problem is tougher than that … It will require attack from several fronts. Which variables should be measured, which inputs should be manipulated and which links should be made between the two sets? Such are the questions that need answers, and it is the burden of the new theories to invent ways both of asking and answering these questions in an efficient and organized manner"

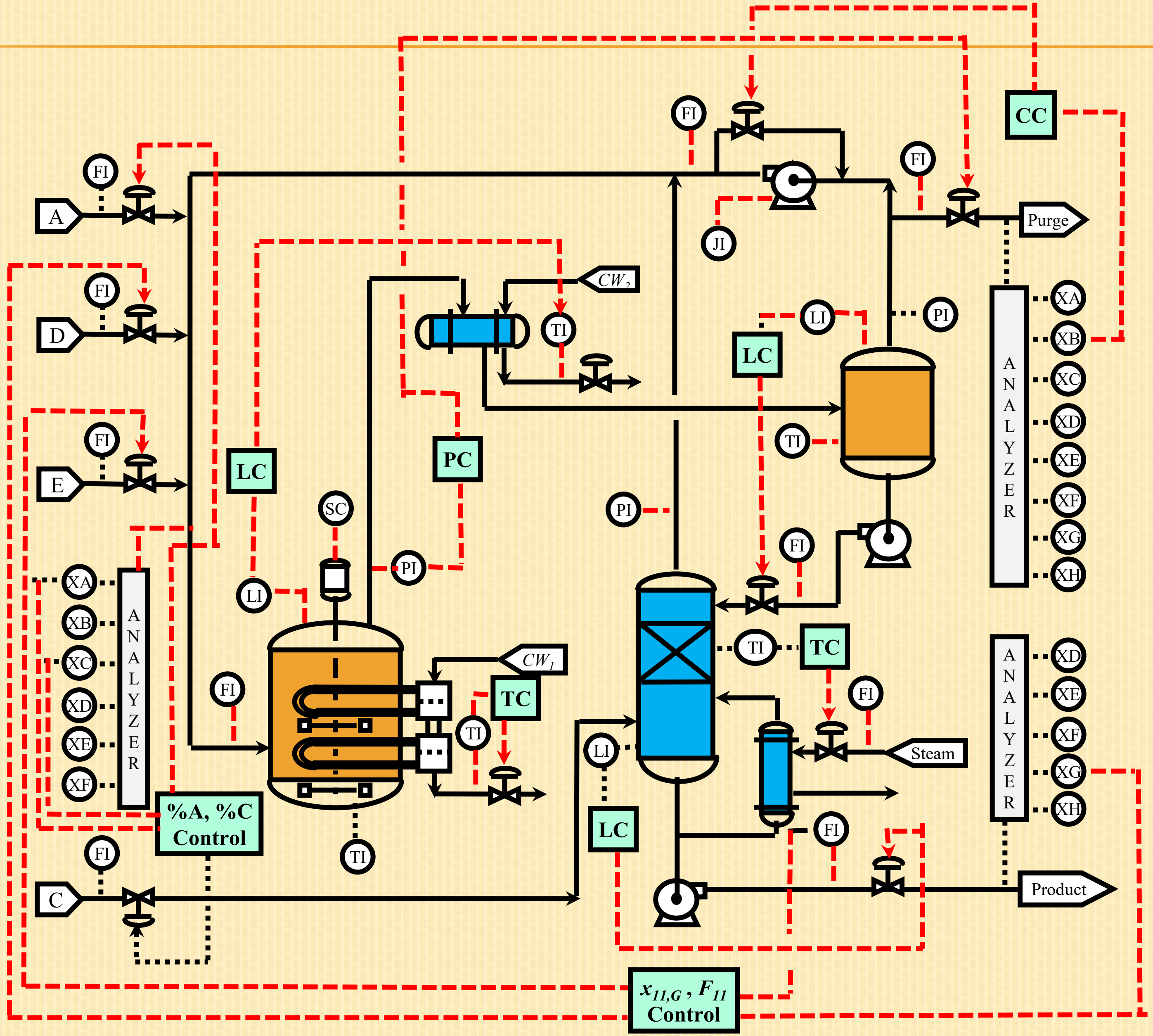
Alan Foss, Critique of Chemical Process Control Theory, 1973

"The problems wear masks, as usually,
and when they do,
it is hard to discern the actual state of the problem
and thus its proper formulation"

"the wronger answer to the righter question,
is better than
the righter answer to the wronger question"

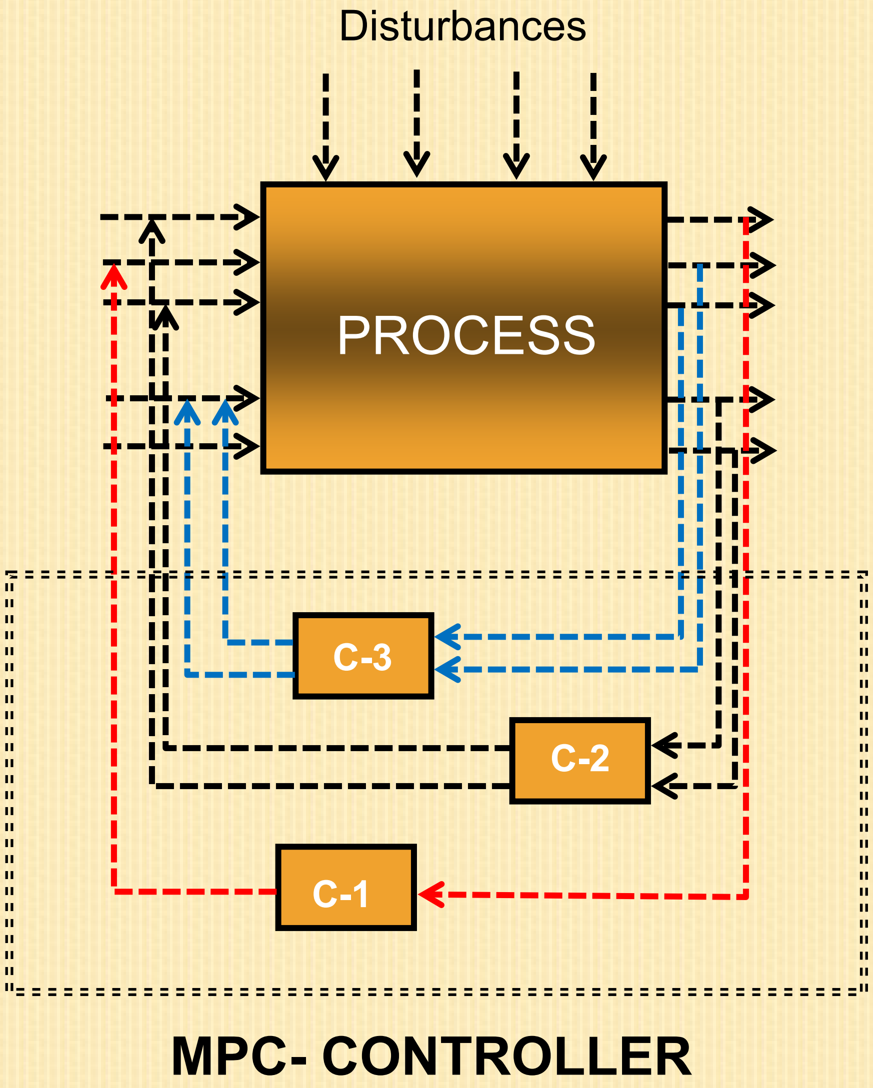
The Tennessee Eastman Chemical Co. Plant



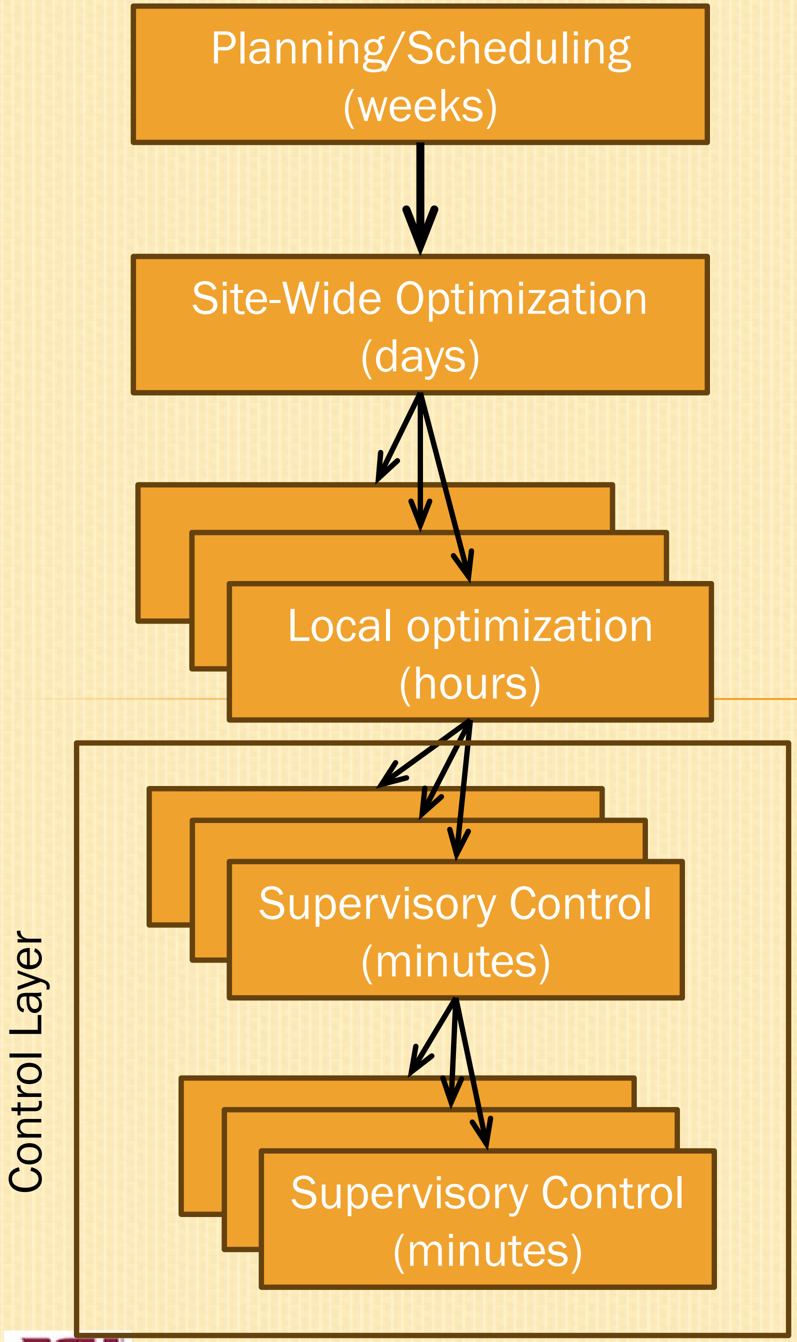


FI
A
D
E
C
XA
XB
XC
XD
XE
XF
XG
XH
ANALYZER
%A, %C Control
LC
PC
SC
LI
PI
TI
TC
CW_1
CW_2
JI
CC
Purge
Steam
Product
$x_{11,G}$, F_{11} Control

Formulation of the Problem: The Open Question



- Select Control Objectives
- Identify the Measured Outputs
  - Associate with Operating Objectives
    - Observability
- Identify Manipulated Inputs
  - Controllable Structures
- Create I/O Model
  - The Least “Expensive” Necessary
- Select the Weights
  - Control Outputs; Manipulated Inputs
- Pose Constraints on
  - Inputs; Outputs
- Design the MPC – Controller
  - Impact of uncertainties
  - Stability; Performance



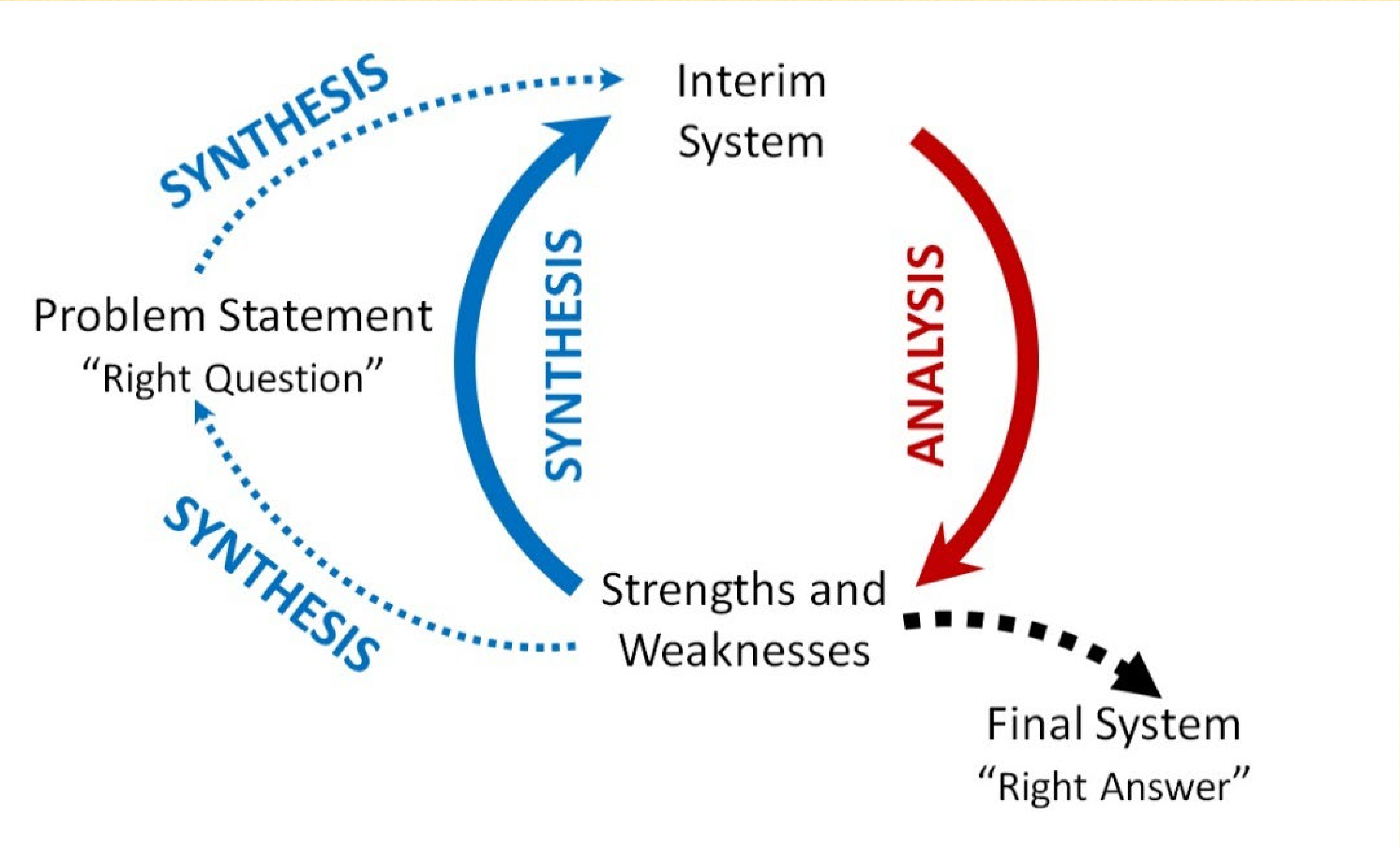
Skogestad Framework

I. Top-down **ANALYSIS**:

- Definition of operational objectives
- Manipulated variables and degrees of freedom
- Primary controlled variables
- Production rate

II. Bottom-up **SYNTHESIS** of the control system:

- Regulatory Control
  - Stabilization
  - Local disturbance rejection
- Supervisory Control
  - Decentralized
  - Multivariable: MPC for the constraints.
- Optimization layer



Every Engineering Design Activity is a Trade-Off Between Information and Cost

“What goes on in the designer’s head is not purely formalizable, either in abstract terms.., or in taxonomic views....

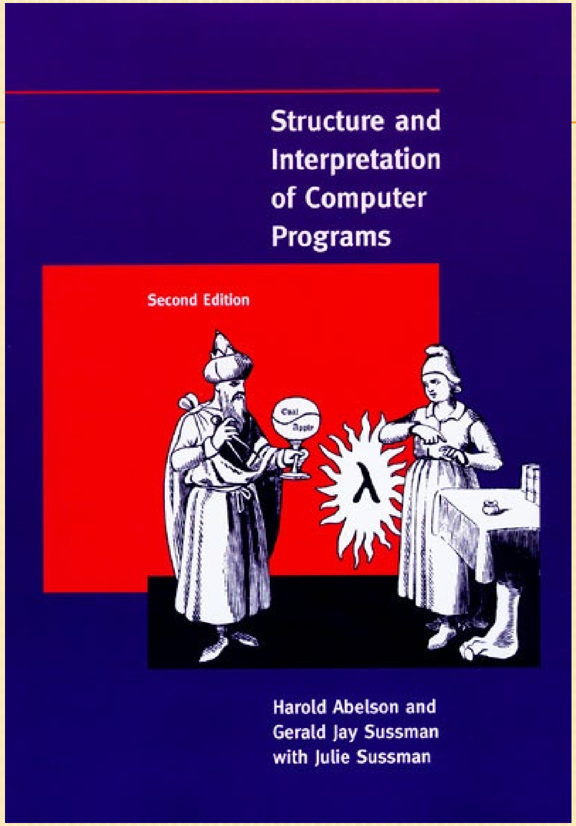
It has structure, it has technique that
can be taught and learned, but
involves also a personal touch, not only in trivialities but
in deeper considerations of skill and suitability ...”

What is the Role of Computers
In the Design of Engineered Systems?

Period 2: MIT(1985-2000)

Becoming student again: Intelligent Systems for Process Engineering

The "Wizard Book"



Symbolics 3640

The first commercially available "Workstation"

LISPE: Laboratory for Intelligent Systems in Process Engineering

Methodologies

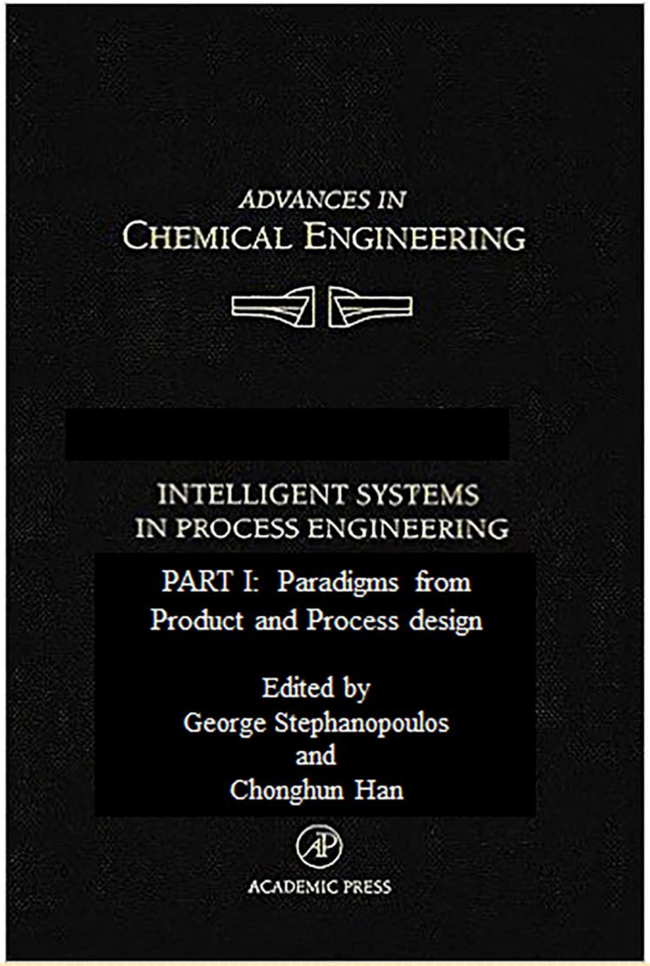
- Automation in design
- Symbolic and order-of-magnitude reasoning
- Inductive and deductive reasoning
- Searching spaces of discrete solutions
- Nonmonotonic reasoning
- Analogical learning
- Empirical learning through multi-scale, hierarchical NN
- Reasoning in time
- Learning Concepts (logical relationships) from numerical computations

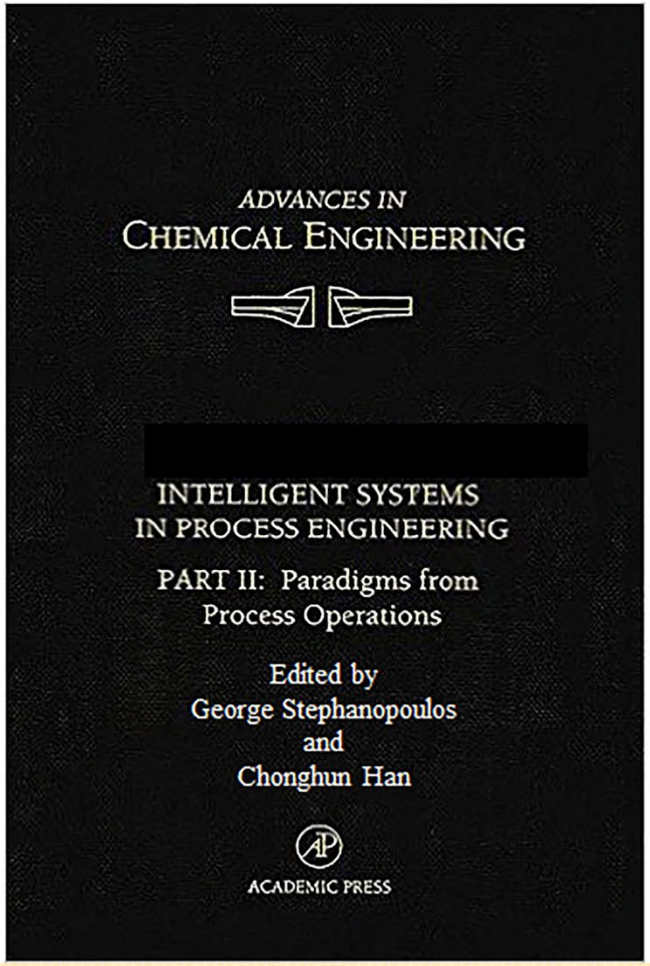
Domain-Specific Problems

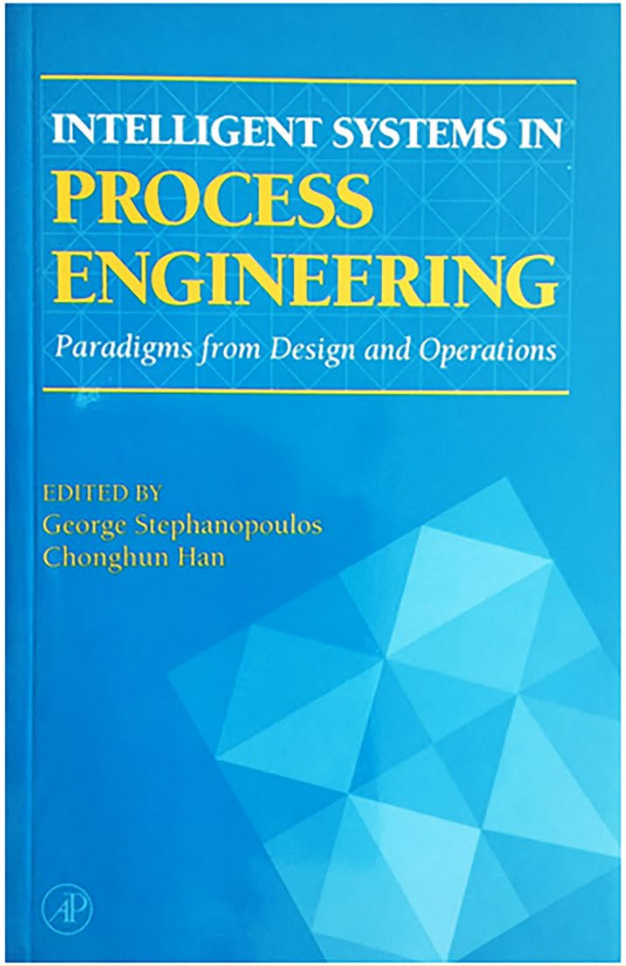
- From reactions to
  - Complete chemical processes
  - New processing concepts
  - Identification of process hazards
- Design of Plant-Wide Control Structures
- Synthesis of biochemical networks
- Design of molecules with desired properties
- Synthesis of operating procedures
- Fault detection and diagnosis
- Batch to batch process improvements

INTELLIGENT SYSTEMS IN PROCESS SYSTEMS ENGINEERING

(ACADEMIC PRESS, DECEMBER 1995)

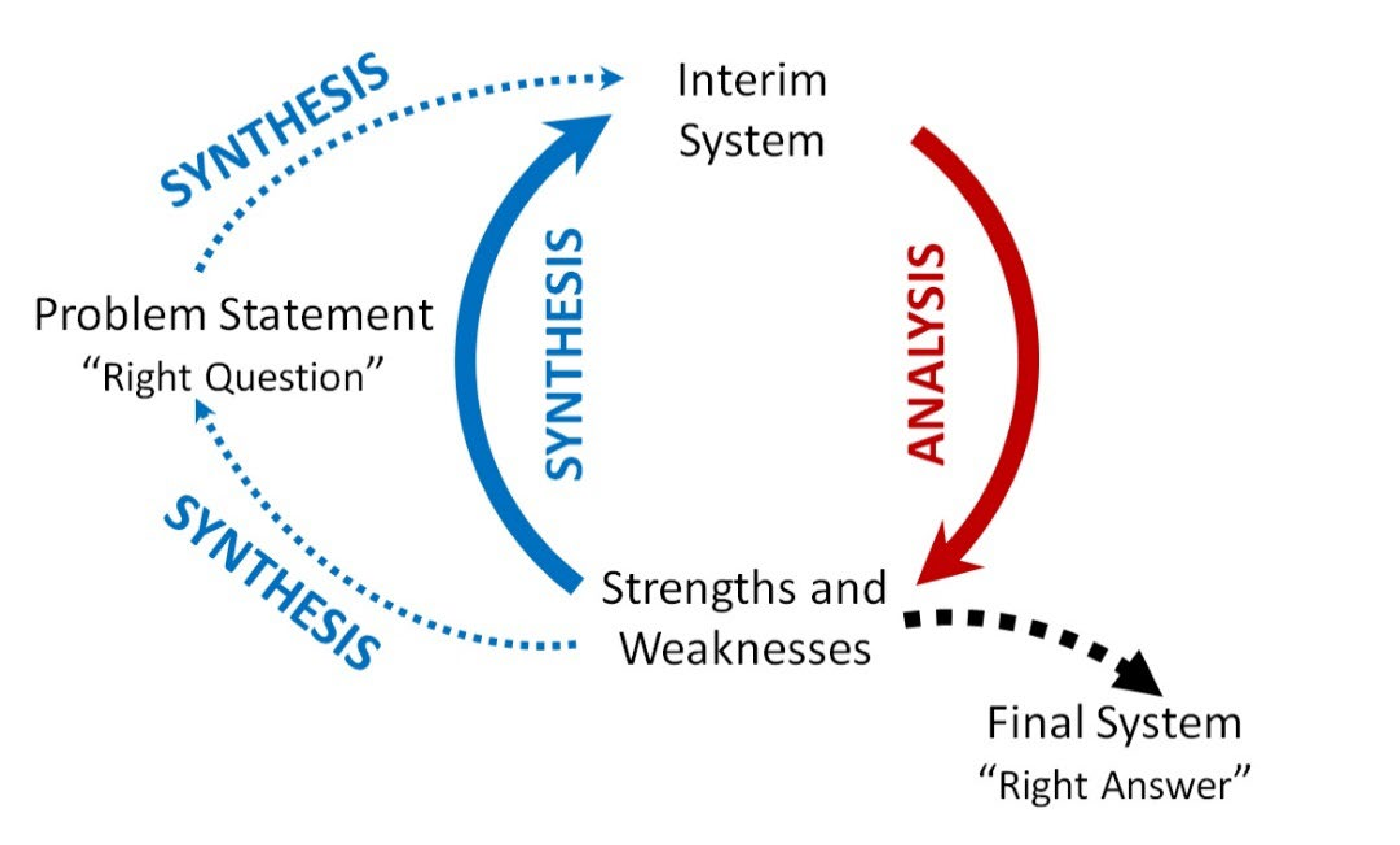




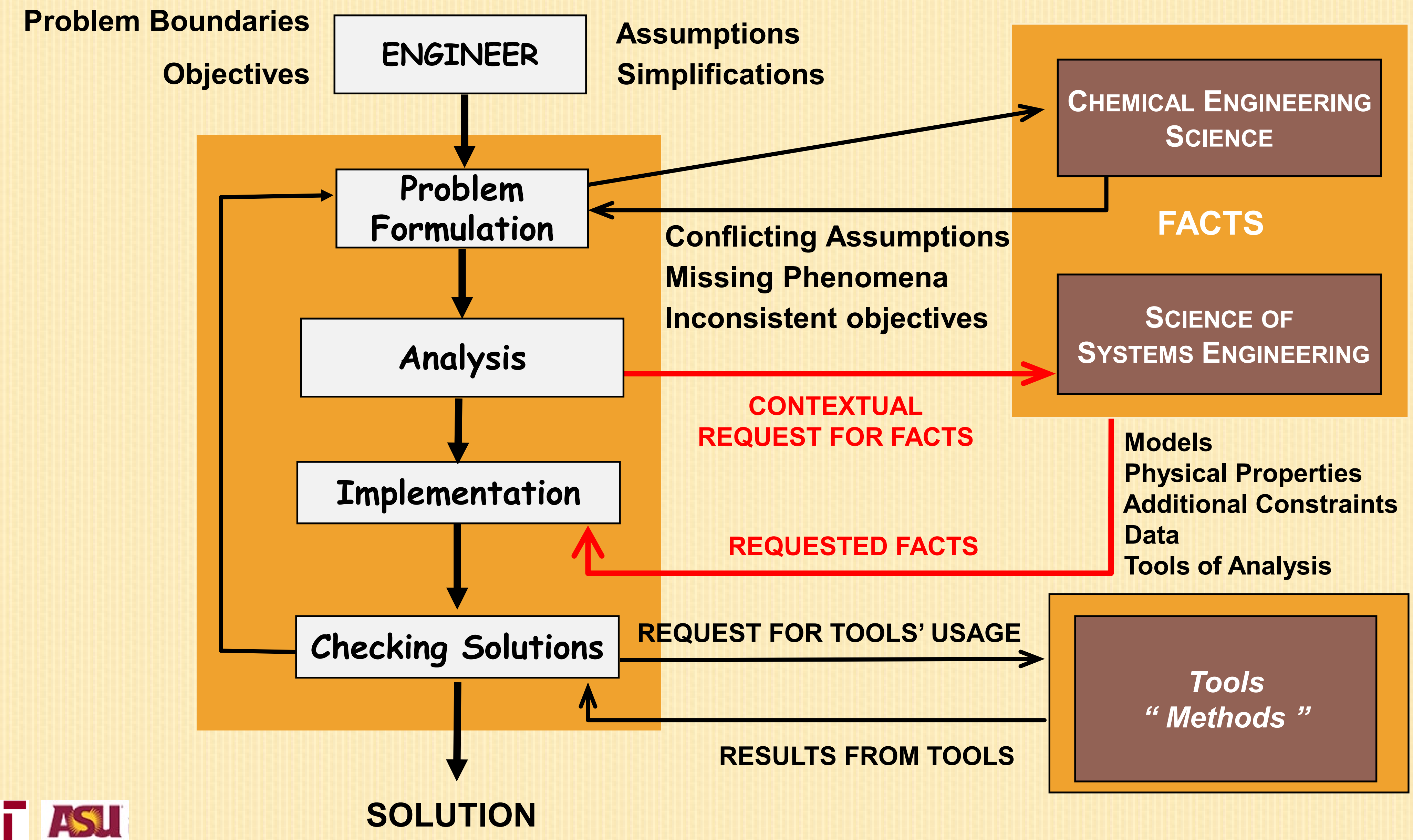


1. Integration of Humans and Computers in design activities

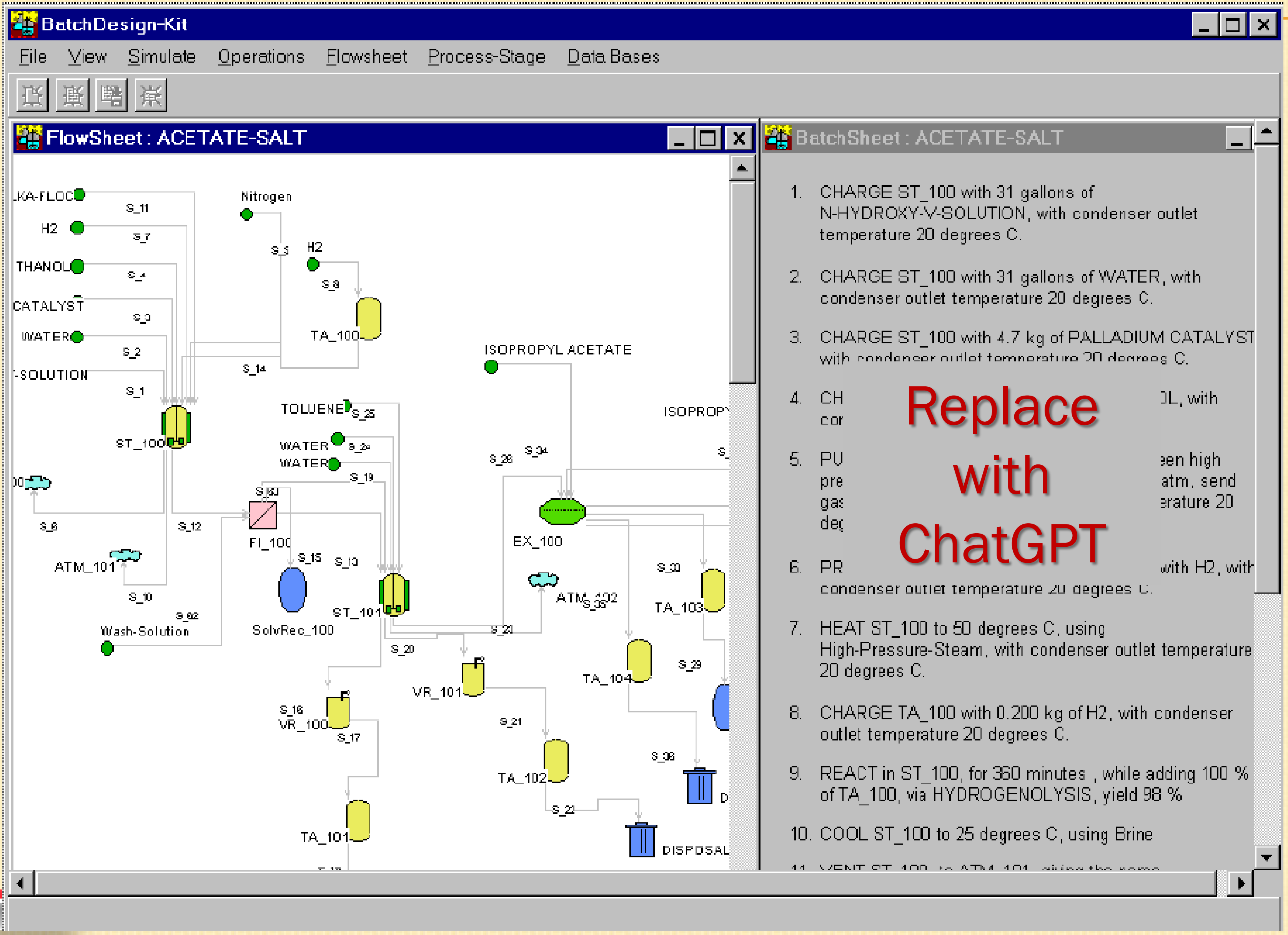
2. Learning Properties of Algorithms from Computational results



Interim System
SYNTHESIS
SYNTHESIS
ANALYSIS
Problem Statement
"Right Question"
SYNTHESIS
Strengths and Weaknesses
Final System
"Right Answer"


Problem Boundaries
Objectives
ENGINEER
Assumptions
Simplifications
Chemical Engineering Science
FACTS
Science of Systems Engineering
Problem Formulation
Analysis
Implementation
Checking Solutions
Conflicting Assumptions
Missing Phenomena
Inconsistent objectives
CONTEXTUAL REQUEST FOR FACTS
Models
Physical Properties
Additional Constraints
Data
Tools of Analysis
REQUESTED FACTS
REQUEST FOR TOOLS' USAGE
Tools
" Methods "
RESULTS FROM TOOLS
SOLUTION

(BATCH DESIGN-KIT)

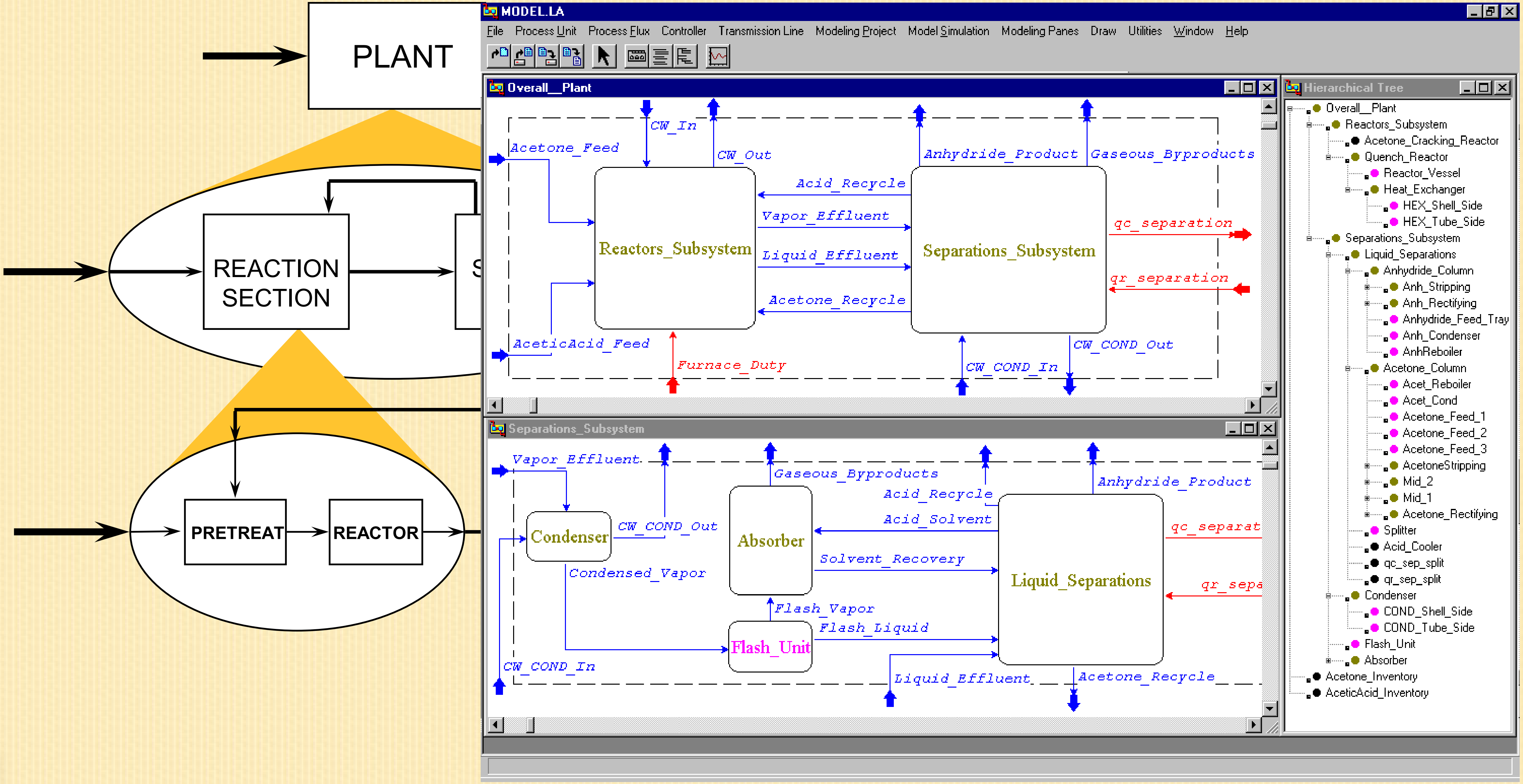


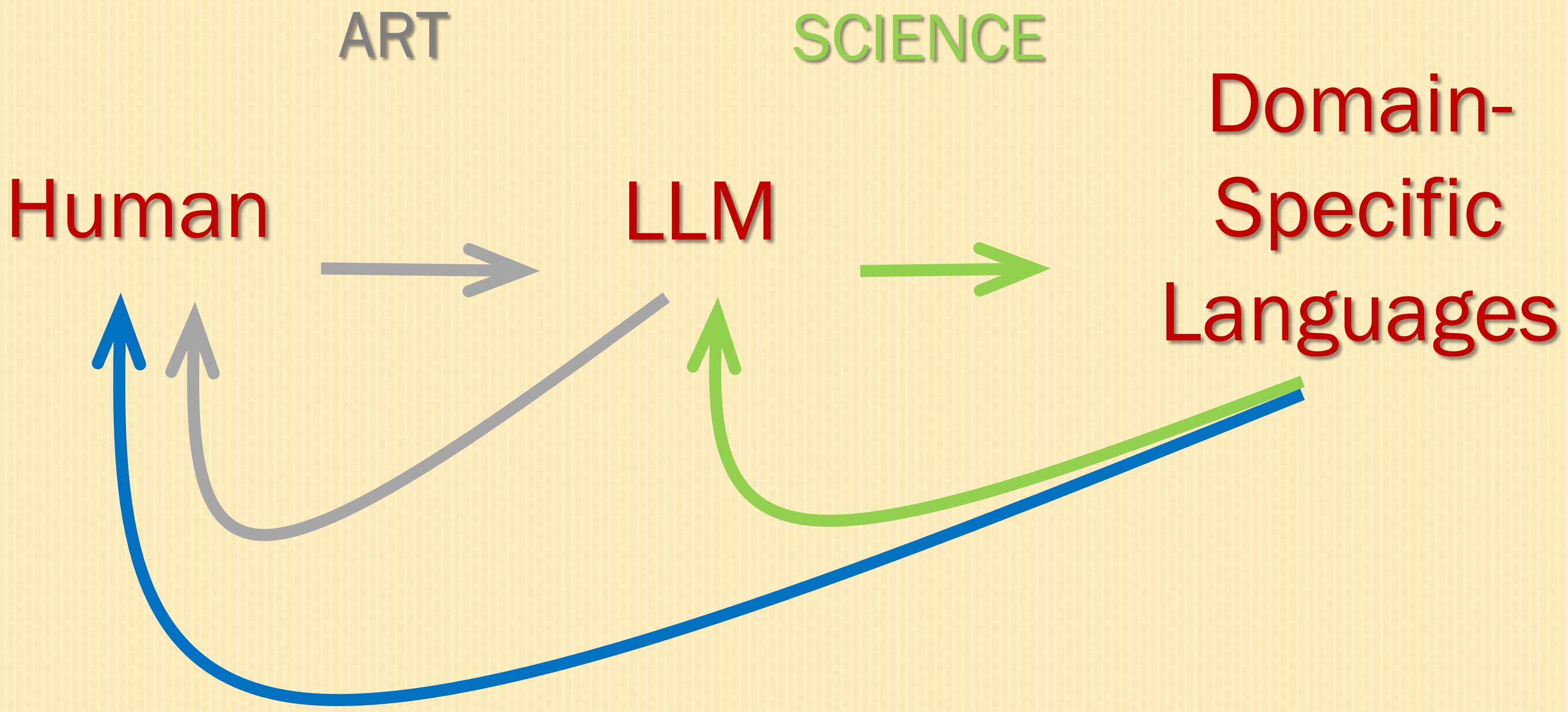
Replace with ChatGPT

Behind the Scene using the Modeling Language

- Generate Constraints?
- Consistency-Conflicts?
- Regulations?
  - US, EU, Japan
- Violations?
  - Environmental
  - Economic
  - Health
  - Operating
- Alerts
  - Improvements
- Explanations
- Next steps

MODEL.LA: HIERARCHICAL MODELING





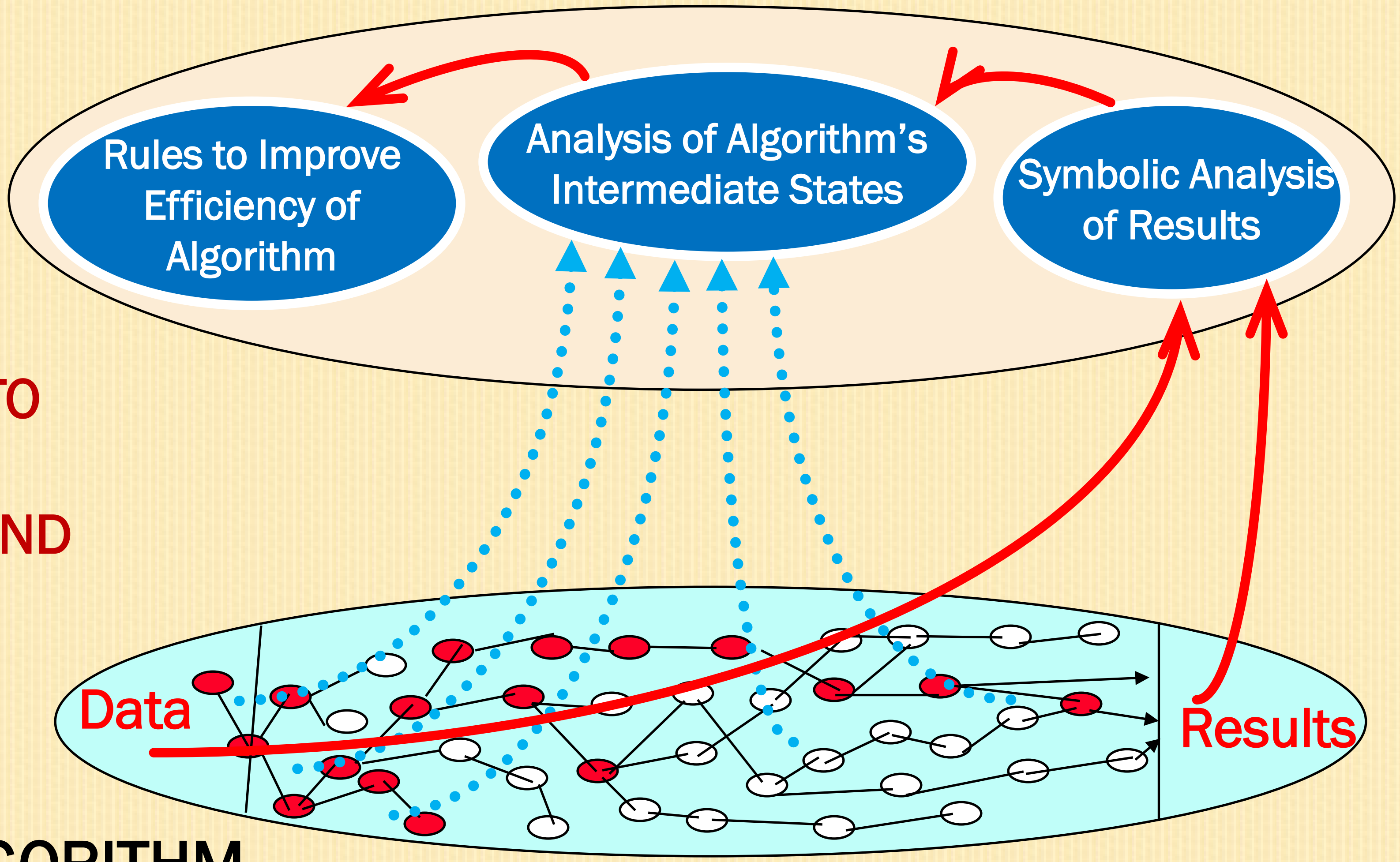
Common Thread: Knowledge Representation

→ MODELING LANGUAGES

Scientific Computing and Machine Learning

SUPERVISORY LOGIC
(Explanation-Based Learning)

LEARNING HOW TO IMPROVE BRANCH-AND-BOUND ALGORITHMS



NUMERICAL ALGORITHM
(Branch-and-Bound Algorithm)

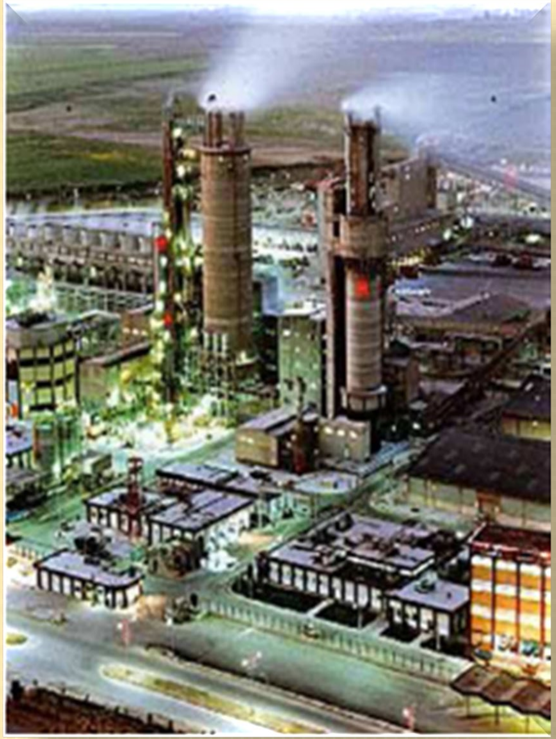
Period 3: Mitsubishi Chemical Corporation (2000-2005)

The most fascinating voyage of my life

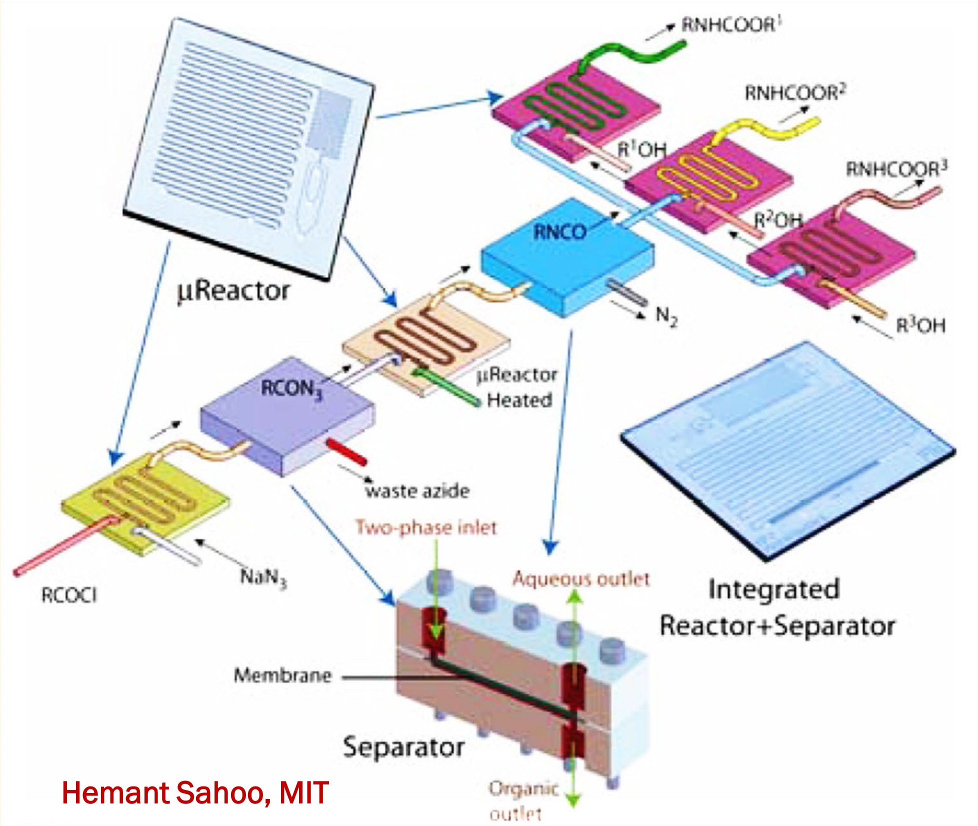
Period 4: MIT(2005-2015)

Becoming student again:
Statistical Mechanics and Control

FROM MACRO- TO MICRO-SCALE PROCESSING

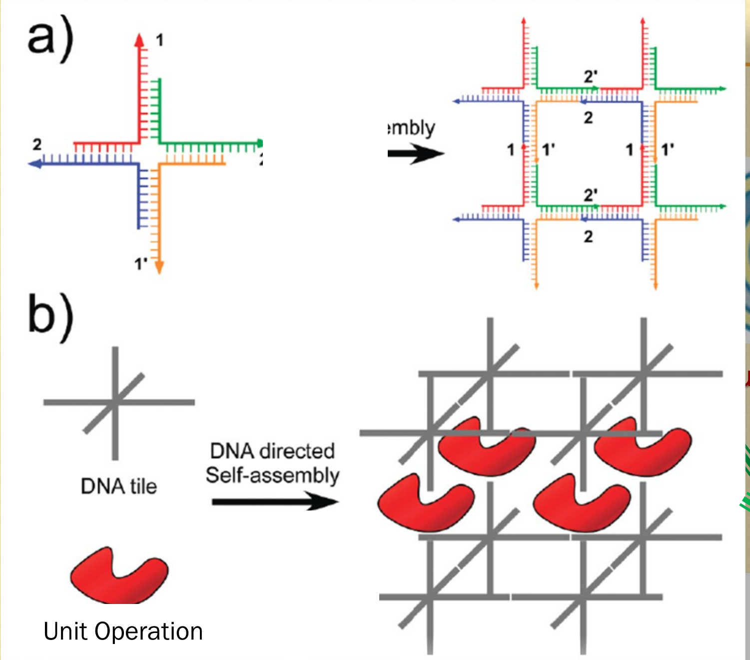


Macro-Scale processing



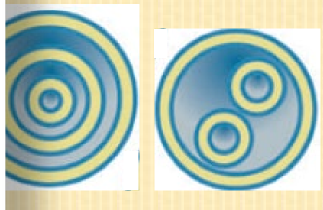
Micro-Scale processing

Synthetic Nanoscale Processing System

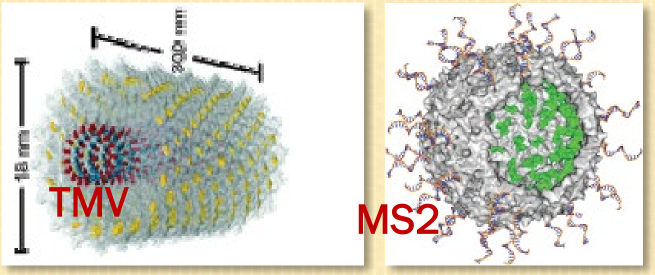


Scaffoldings:
Directed Self-Assembly of DNA Tiles

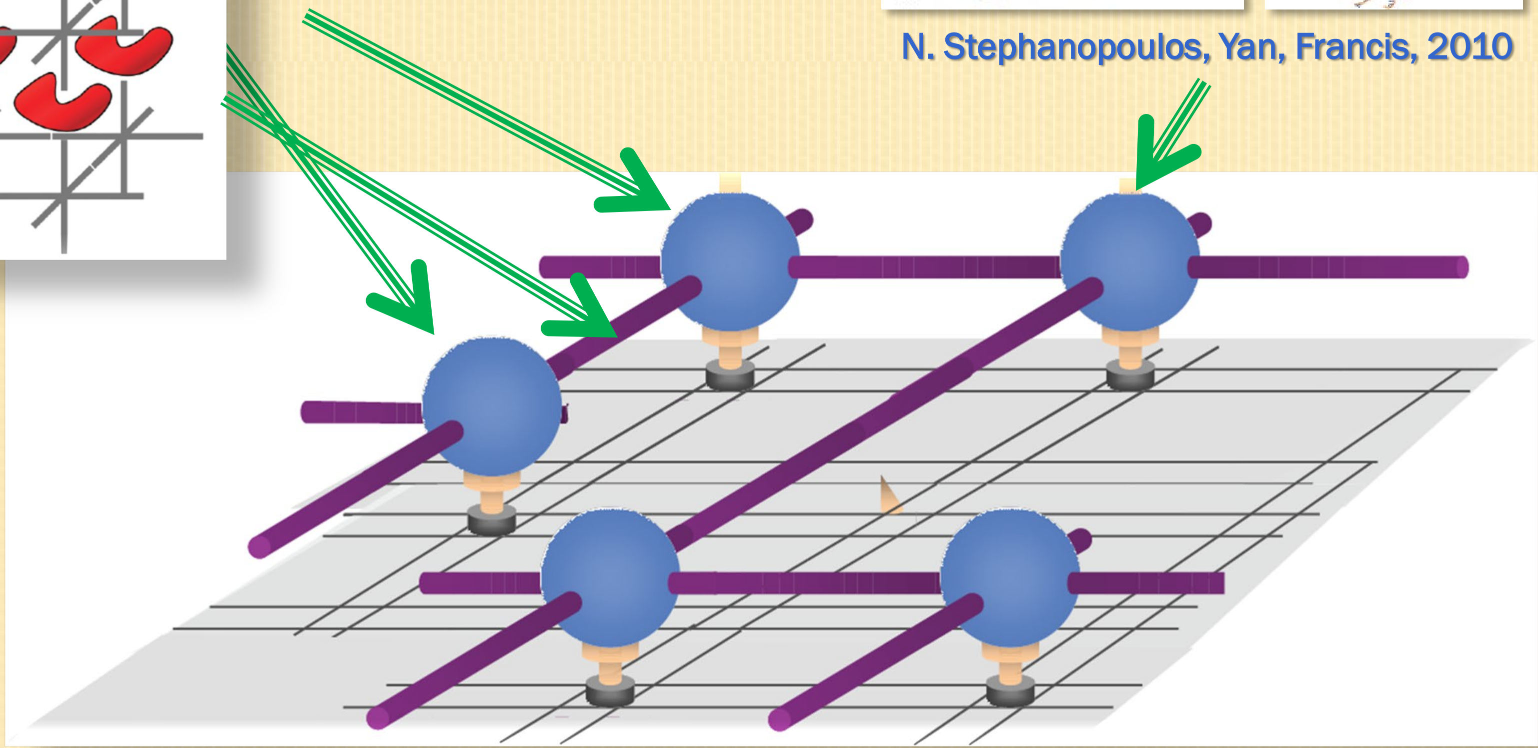
PACE, 2010



Viruses



N. Stephanopoulos, Yan, Francis, 2010



N. Stephanopoulos, E. Solis, G. Stephanopoulos, *AIChE Journal, 2005*
Nanoscale Process Systems Engineering: Toward Molecular Factories, Synthetic Cells, and Adaptive Devices.

COMPONENTS OF MOLECULAR MANUFACTURING SYSTEMS

- "Unit Operations" at the Nano-Scale
  - Reactors; of many different shapes and characteristics
  - Separators; channels, pores, gates, molecular sorters, etc.
  - Molecular Mixers, Splitters, etc.
- "Material Transporters" at the Nano-Scale
  - Nanotubes; with chemically-induced mobility
  - Molecular Pumps, Motors, Shuttles, Actuators, etc.
- "Monitoring and Control Elements" at the Nano-Scale
  - Sensors-Signal Carriers:

    Molecular electrical wires;

    Directional gradients of surface charges, ions, molecules
  - Actuators:

    Molecular Switches, Gates, Valves, Motors, Pumps, Shuttles

Generic Design Problems for NanoScale Processing Systems

Problem 1:

Conceptual Design

Problem 2:

Operations Monitoring and Control

Problem 3:

Fabrication

PART-C:

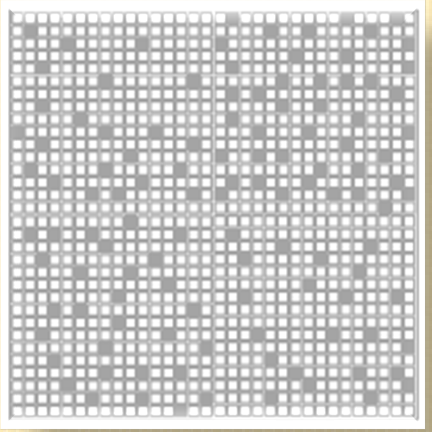
FABRICATION OF NANO-SCALE PROCESSES:

CONTROLLED FORMATION OF NANOSTRUCTURES WITH DESIRED GEOMETRIES

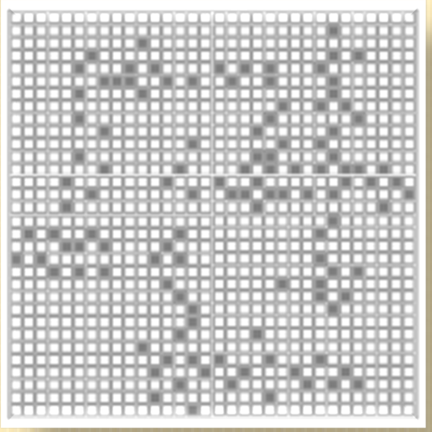
Guided Static Self-Assembly:
Final State "Stable" and "Robust"

Static Problem:

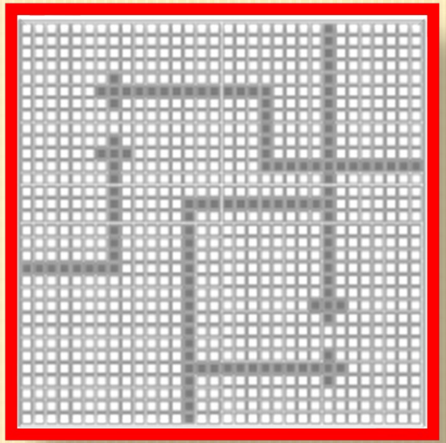
Ensure that the Final State is "Stable" and "Robust"



Initial State: Random Distribution of Particles



Intermediate State: "Desired" Distribution of Particle Numbers



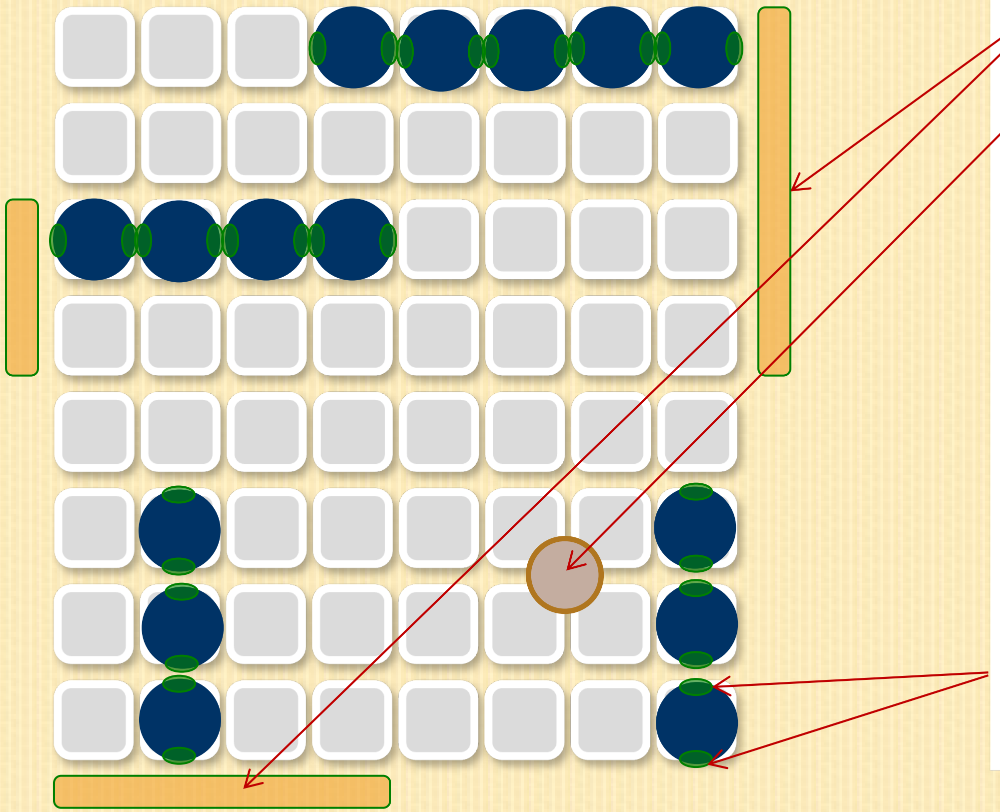
Final State: Structure with Desired Geometry

Dynamic Problem:

Ensure that Final State is reached from any initial state

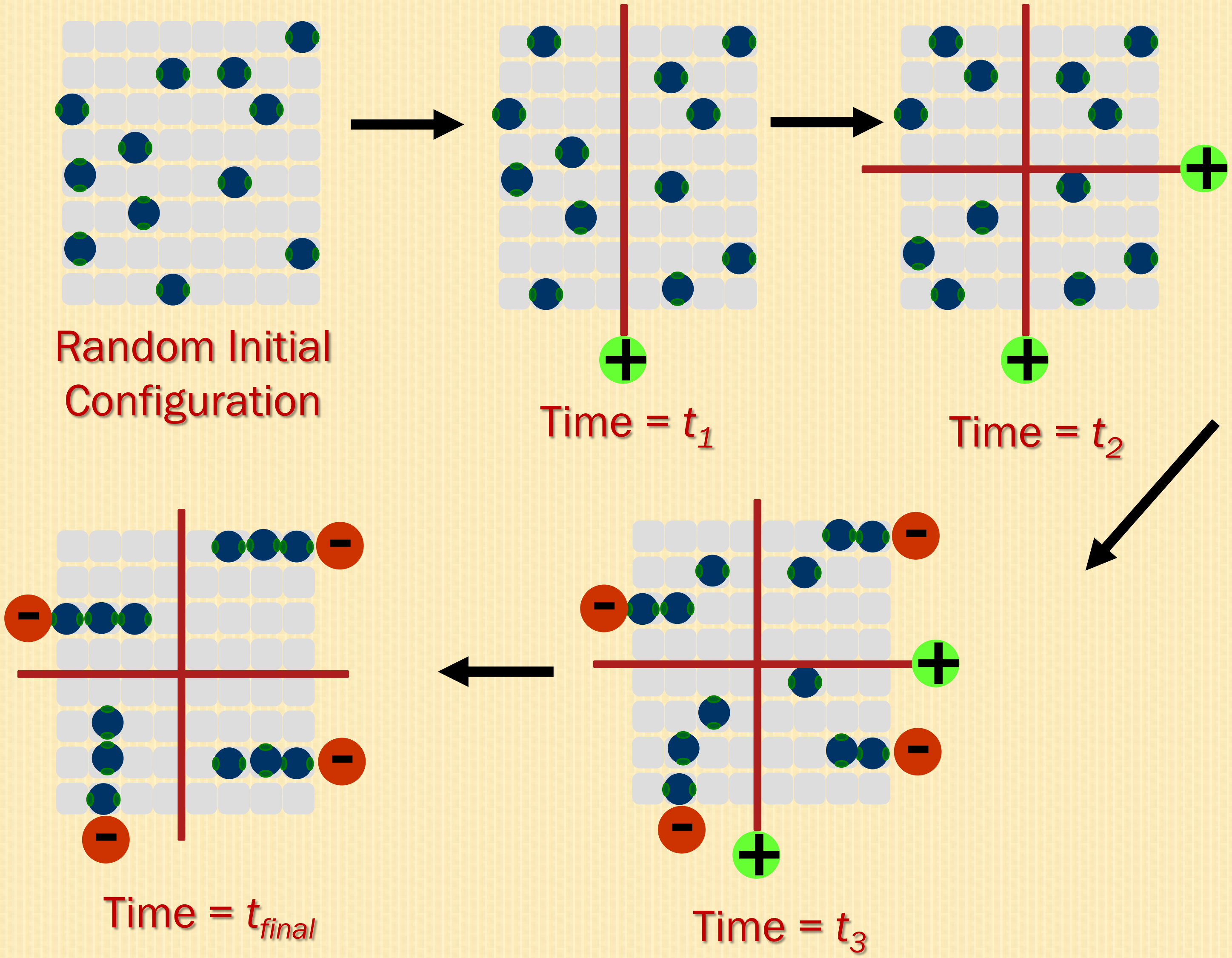
MODEL SYSTEM

Desired Structure

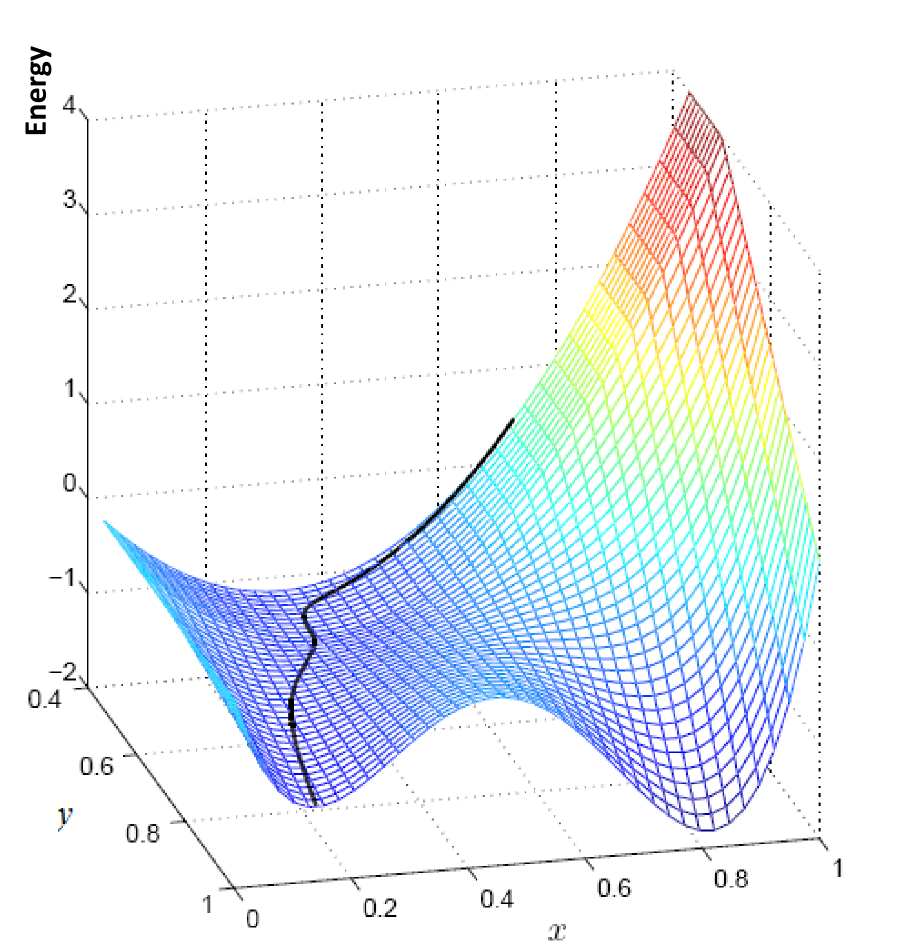


- Boundary Controls
- Internal Point Controls
  - Can adjust location, & intensity
  - Can vary with time
- Temperature
- Medium; Solvent
- Molecular Controls
  - Particle Size, Shape and Functionality

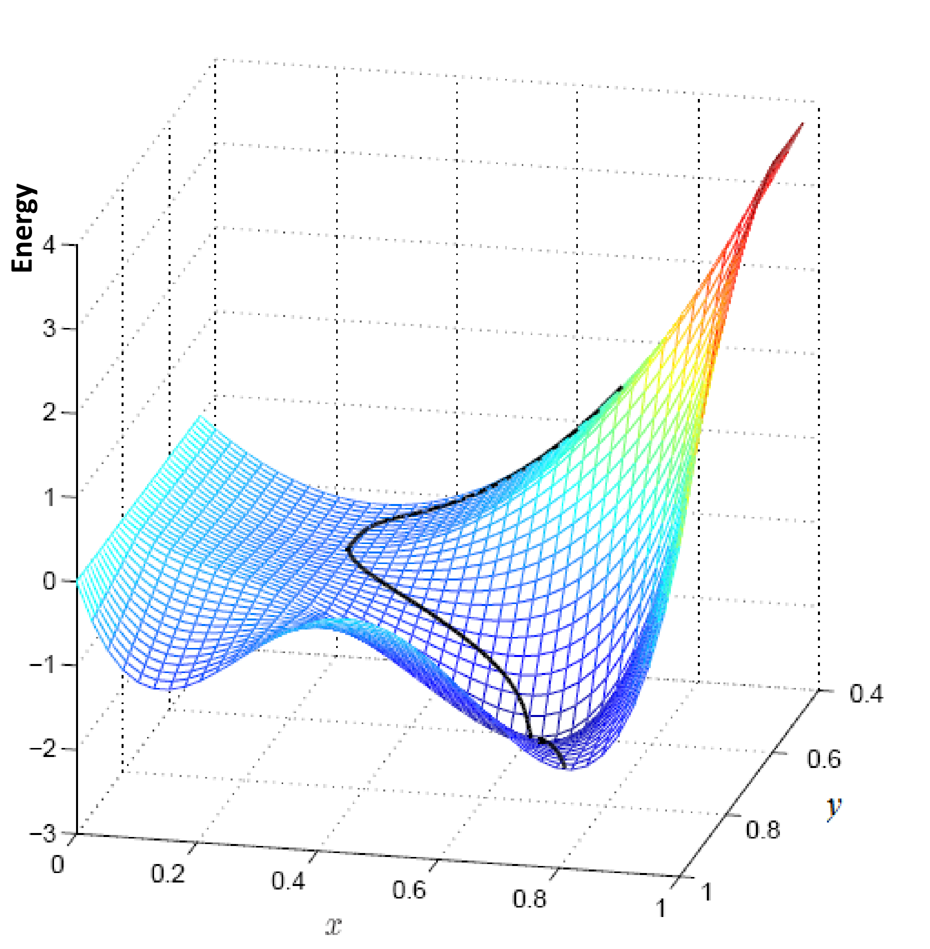
Controlling Complexity by Breaking Ergodicity: Progressive Refinement of Compositional Configurations



GUIDED DYNAMIC SELF-ASSEMBLY:

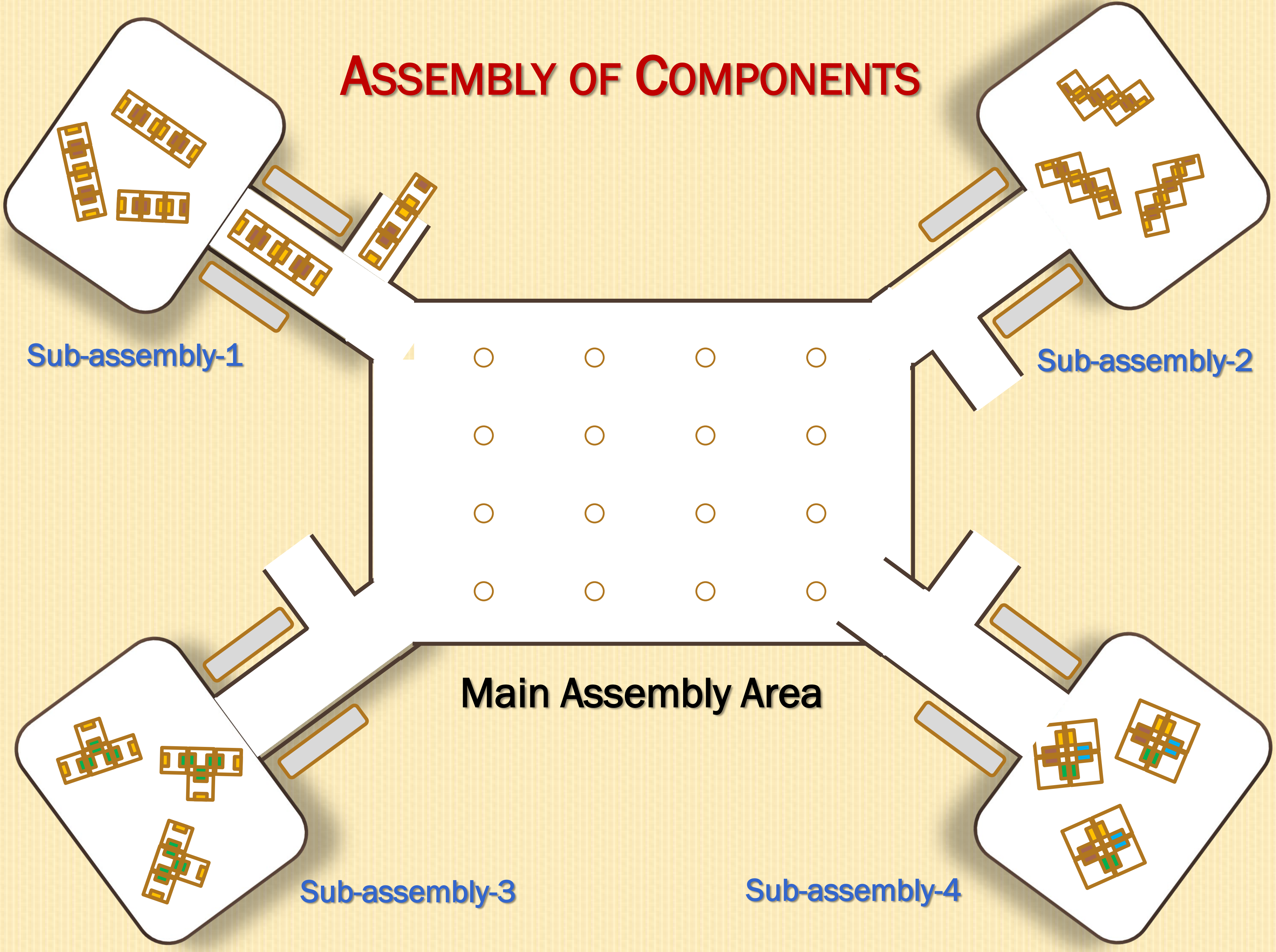


Undesired path



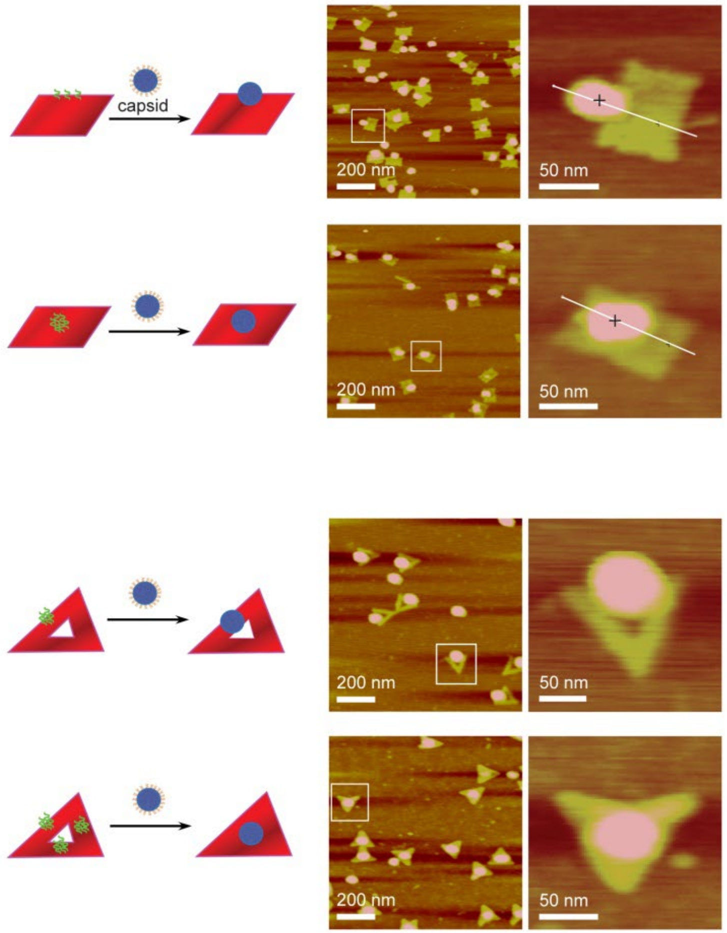
Desired path

Assembly of Components

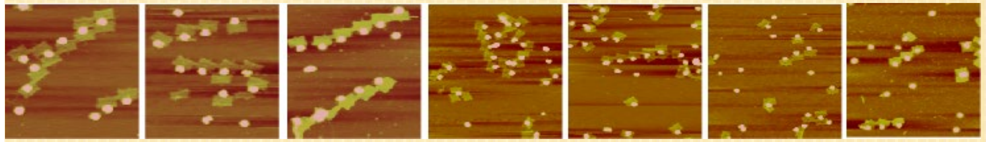


EXPERIMENTAL VERIFICATION

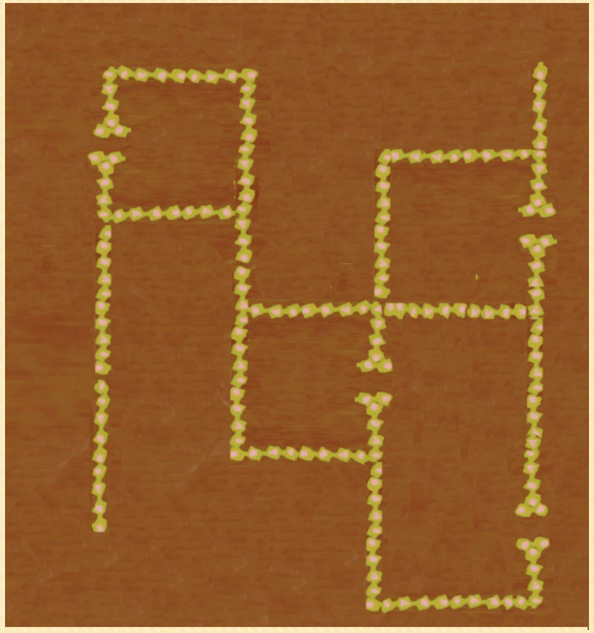
single tile results (these are all AFM images):



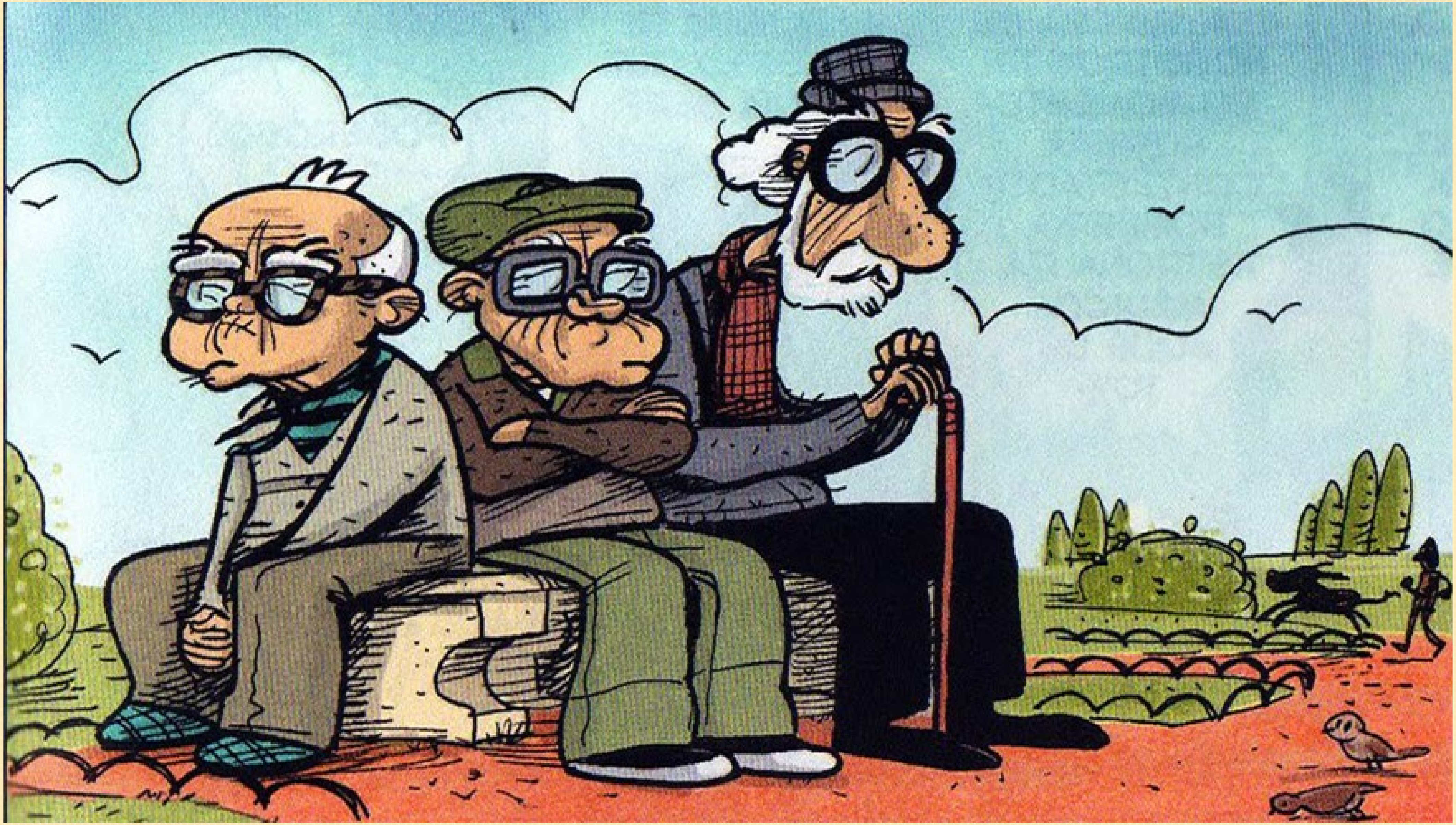
the efficiency of capsid-tile association is very high, approaching 100%



Before



After



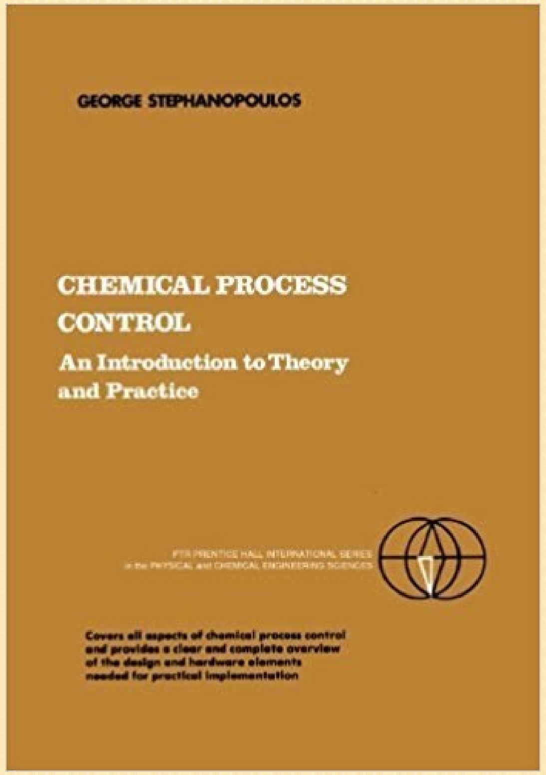
QUINO (Joaquín Salvador Lavado)

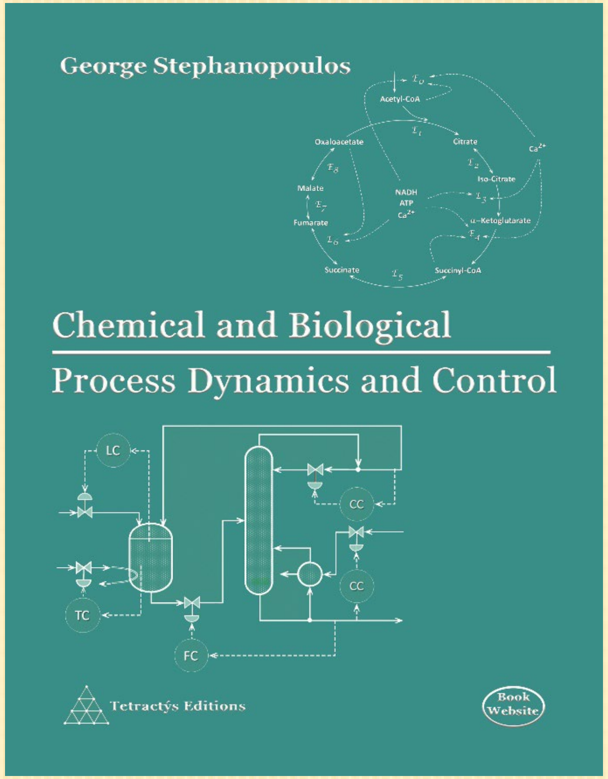
QUINO

Period 5: MIT(2015-now)

writing a book on
Chemical and Biological Process Dynamics and Control.

(1984)





(2025)

A.W. Westerberg to Geo.S. (1972): Controller = inversion of the model

$$y = f(u,d) = y_{SP} \quad \Rightarrow \quad u = f^{-1}(y_{SP}, d)$$

Fred Bailey (U of Mn) to Manfred Morari (1975)

Why do you need feedback?

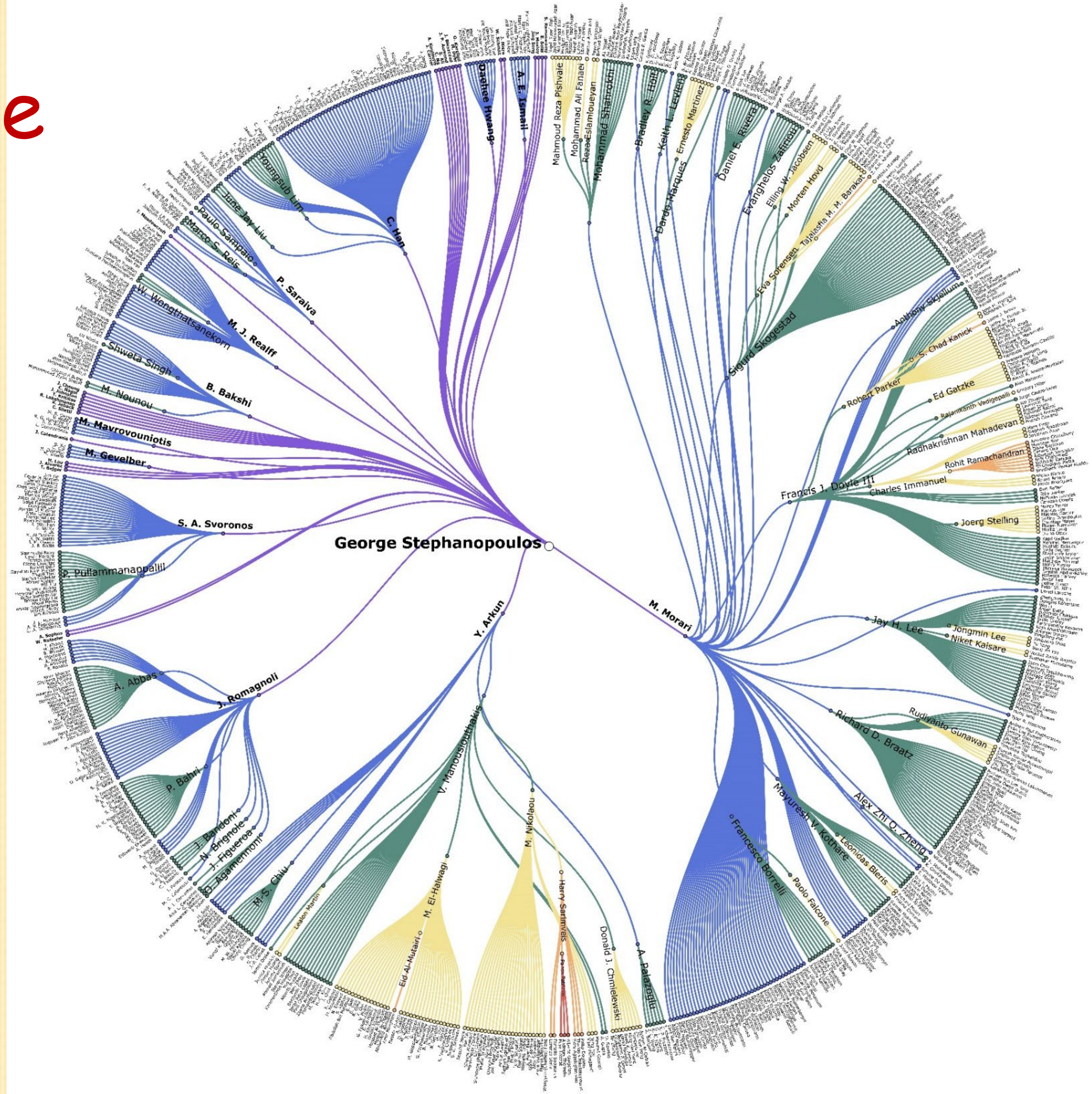
The Internal Model Principle of control theory

- Francis and Wohnam (1976)
- Bengtsson (1977)
- Morari and Garcia (1982)

Chemical and Biological Process Dynamics and Control

- Integrates chemical/biochemical processing systems and biomolecular networks.
- Approaches the design of control systems in three(3) stages:
  - Stage 1: **Structural** Analysis: Control configurations.
  - Stage 2: **Steady State** Analysis: Operability; Steady State Controllers; square and non-square systems.
  - Stage 3: **Dynamic** Analysis: The design of Dynamic Controllers.
- Articulates the foundational principles of feedback control
  - Every feedback controller is based on an internal model
  - The "Nominal" control is an approximation of the inverse of the internal model
    - If performance of the "Nominal" is not acceptable, stop. Go back and do something to improve the model.
    - For setpoint tracking and disturbance rejection you need 2 degrees of freedom.
  - The stability of the closed-loop response with "Nominal" controller, depends solely on the magnitude of the modeling error.
  - The performance of the "Nominal" controller, depends on the magnitude of the modeling error and it is always a subjective decision.
- Unified treatment of controller design methodologies from PID to MPC.
- Unifies continuous-time and discrete-time.
- All analysis and design is in the time domain.

Gratitude



Academic Family Tree