Hybrid Algorithms for Stochastic Integer Programs in Chemical Batch Scheduling

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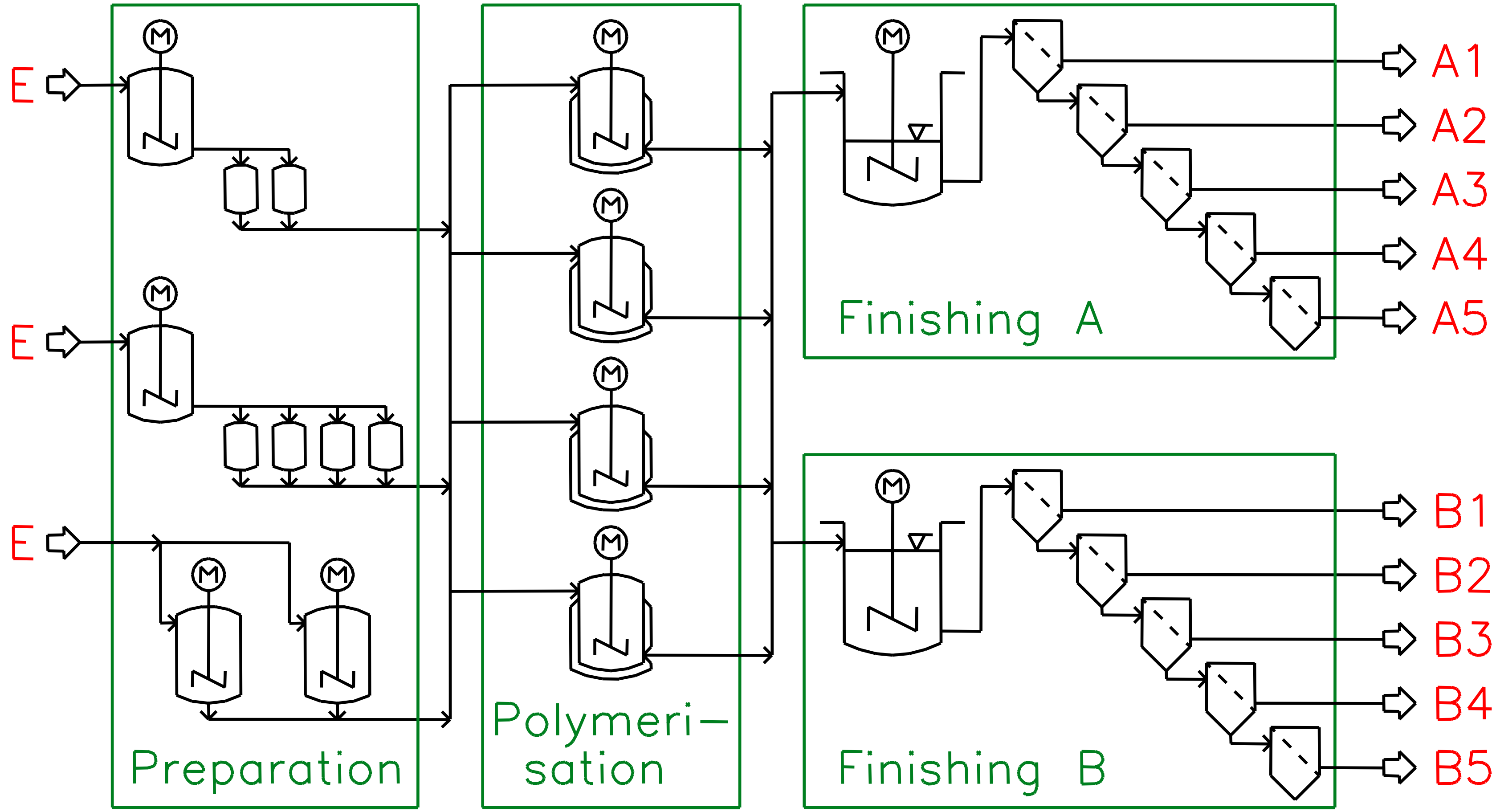
OUTLINE

1. **CHEMICAL BATCH SCHEDULING**
2. **STOCHASTIC INTEGER PROGRAMS**
3. **HYBRID EVOLUTIONARY ALGORITHMS**
   - General Evolution Strategy
   - Specific Evolutionary Algorithm
   - Comparative Numerical Tests

Chemical Batch Scheduling

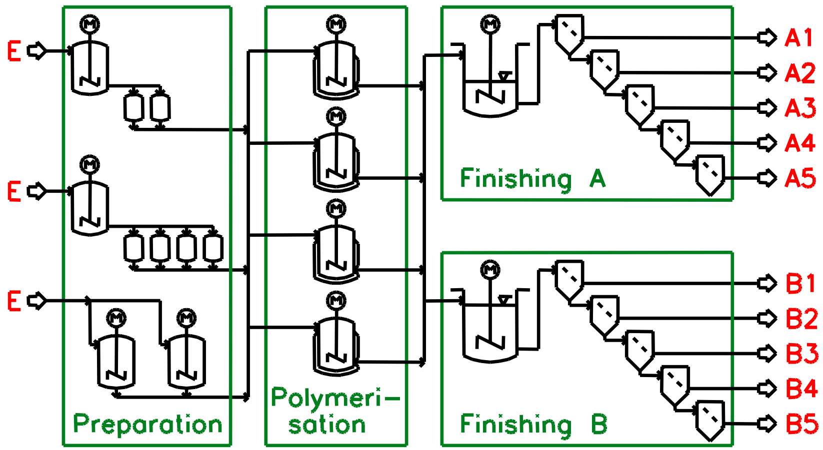
- **Given**
  - Flexible multi-product batch plant
  - Recipes for batch-wise production
- **Batch Scheduling**
  - Feasible and optimal assignment of processing steps – plant units – time
- **Mixed-Integer Linear Program (MILP)**
- **Real-Time Conditions**
  - Uncertain data: large-scale problems
  - Limited solution time: fast algorithms

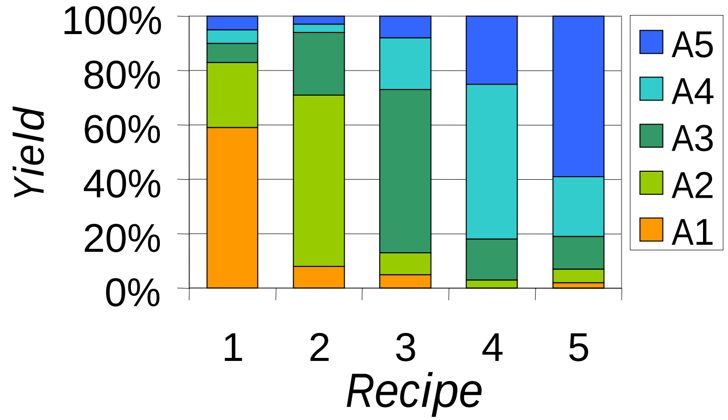
EPS-Production



Aggregated Scheduling Model

- **Moving horizon**
- **Discrete decisions**
  - Number, timing and recipes of batches
  - Operation *Finishing*
- **Constraints**
  - Capacity *Polymerization*
  - Capacity *Finishing*
  - Dynamics *Finishing*
- **Economic objective**
- **Uncertainties**
  - Demand
  - Capacity *Polymerization*





Deterministic Base Model

$$\max \sum_{p=1}^{P}\left(\sum_{l=1}^{L}\sum_{i=1}^{I}\sum_{f_p=1}^{F_p}\alpha_{lif_p}M_{lif_p}-\sum_{i=1}^{I}\sum_{f_p=1}^{F_p}\alpha^{+}_{if_p}M^{+}_{if_p}-\sum_{i=1}^{I}\sum_{f_p=1}^{F_p}\alpha^{-}_{if_p}B^{-}_{if_p}-\sum_{i=1}^{I}\sum_{r_p=1}^{R_p}\beta_{ir_p}N_{ir_p}-\sum_{i=1}^{I+1}\gamma_{ip}w_{ip}\right)$$

profit

$$s.t. \quad \sum_{l=1}^{L}\begin{cases}M_{l(i+l-1)f_p} & \text{if } i+l-1\le I\\ 0 & \text{else}\end{cases} = B^{cus}_{if_p}-B^{-}_{if_p} \quad \forall i,f_p \mid i\le I$$

demand

$$\sum_{j=1}^{i}\sum_{l=1}^{L}\begin{cases}M_{ljf_p} & \text{if } j\ge l\\ 0 & \text{else}\end{cases} \le \sum_{j=1}^{i}\sum_{r_p=1}^{R_p}\bar{\rho}_{f_p r_p}N_{jr_p} \quad \forall i,f_p \mid i\le I$$

supply

$$M^{+}_{if_p} \ge \sum_{j=1}^{i}\sum_{r_p=1}^{R_p}\bar{\rho}_{f_p r_p}N_{jr_p}-\sum_{j=1}^{i}B^{cus}_{if_p} \quad \forall i,f_p \mid i\le I$$

oversupply

$$w_{ip} \ge \begin{cases}z^{0}_{p} & \text{if } i=1\\ z_{(i-1)p} & \text{else}\end{cases} - z_{ip} \wedge w_{ip} \ge z_{ip}-\begin{cases}z^{0}_{p} & \text{if } i=1\\ z_{(i-1)p} & \text{else}\end{cases} \quad \forall i,p$$

state-change finishing lines

$$\sum_{j=i}^{k}\sum_{p=1}^{P}\sum_{r_p=1}^{R_p}N_{jr_p} \le N^{max}_{ik} \quad \forall i,k \mid i\le k\le I$$

capacity polymerization

$$\sum_{j=i}^{k}\sum_{r_p=1}^{R_p}N_{jr_p} \le v_{kp}C^{max}_{p}-\begin{cases}C^{0}_{p} & \text{if } i=1\\ v_{(i-1)p}C^{min}_{p} & \text{else}\end{cases}+\sum_{j=i}^{k}z_{jp}F^{max}_{p} \quad \forall i,k,p \mid i\le k\le I$$

max capacity finishing lines

$$\sum_{j=i}^{k}\sum_{r_p=1}^{R_p}N_{jr_p} \ge v_{kp}C^{min}_{p}-\begin{cases}C^{0}_{p} & \text{if } i=1\\ v_{(i-1)p}C^{max}_{p} & \text{else}\end{cases}+\sum_{j=i}^{k}z_{jp}F^{min}_{p} \quad \forall i,k,p \mid i\le k\le I$$

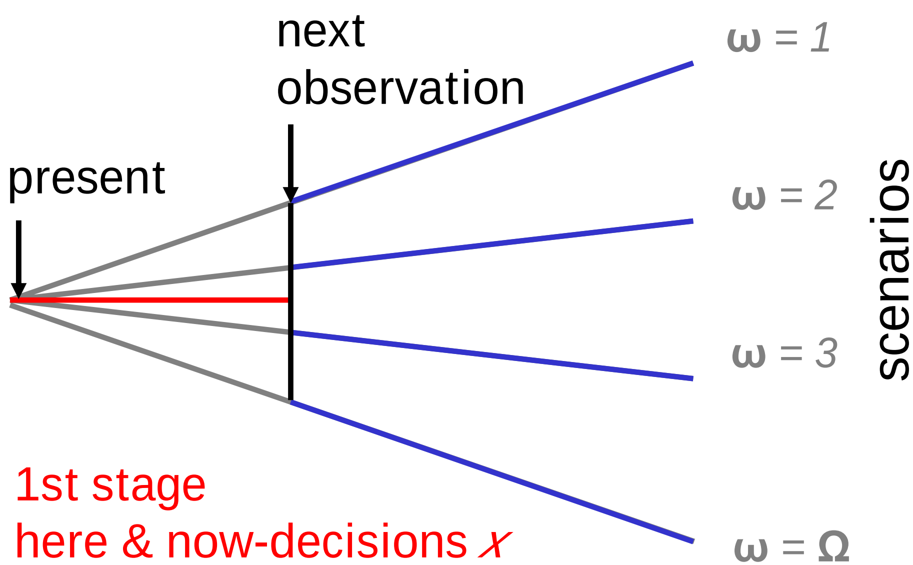
min. capacity finishing lines

$$v_{ip}\le z_{ip} \wedge v_{ip}\le z_{(i+1)p} \wedge v_{ip}\ge z_{ip}+z_{(i+1)p}-1 \quad \forall i,p \mid i\le I$$

$$z_{ip}\in\{0;1\},\quad N_{ir_p}\in IN,\quad M_{lif_p}, M^{+}_{if_p}, B^{-}_{if_p}, w_{ip}, v_{ip}\in IR_{+}$$

STOCHASTIC INTEGER PROGRAMS

- **INFORMATION- AND DECISION STRUCTURE**



1st stage
here & now-decisions x

2nd stage
recourse decisions y_ω

- **DETERMINISTIC EQUIVALENT**

$$
\begin{aligned}
\min_{x,y_\omega} \quad & c^T x + \sum_{\omega=1}^{\Omega} \pi_\omega q_\omega^T y_\omega \\
s.t. \quad & Ax \le b, \\
& T_\omega x + W_\omega y_\omega \le h_\omega, \\
& x \in X, y_\omega \in Y, \omega = \{1, \ldots, \Omega\}, \\
& X, Y \in IR \times IN.
\end{aligned}
$$

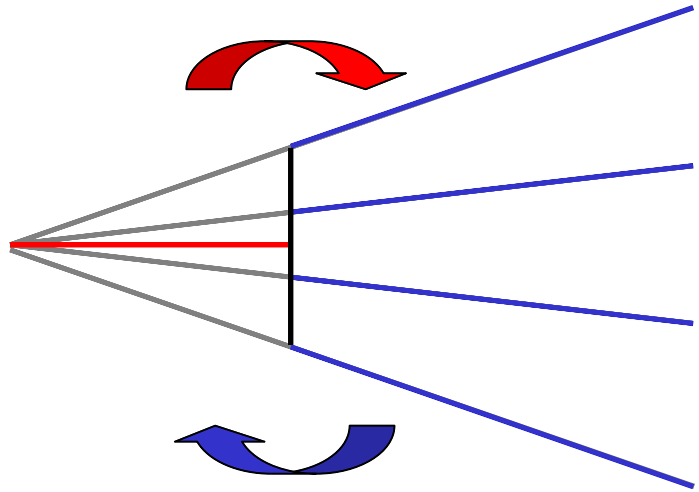
- **MATRIX STRUCTURE**

$$
\begin{bmatrix} A & 0 & 0 & 0 \\ T_1 & W_1 & 0 & 0 \\ \vdots & 0 & \ddots & 0 \\ T_\Omega & 0 & 0 & W_\Omega \end{bmatrix}
\begin{pmatrix} x \\ y_1 \\ \vdots \\ y_\Omega \end{pmatrix}
\le
\begin{pmatrix} b \\ h_1 \\ \vdots \\ h_\Omega \end{pmatrix}
$$

Stage Decomposition

- **Hybrid algorithm**

Evolutionary algorithm: solution candidates x



MILP-algorithm (CPLEX): Objective value (fitness)

Masterproblem: 1st stage

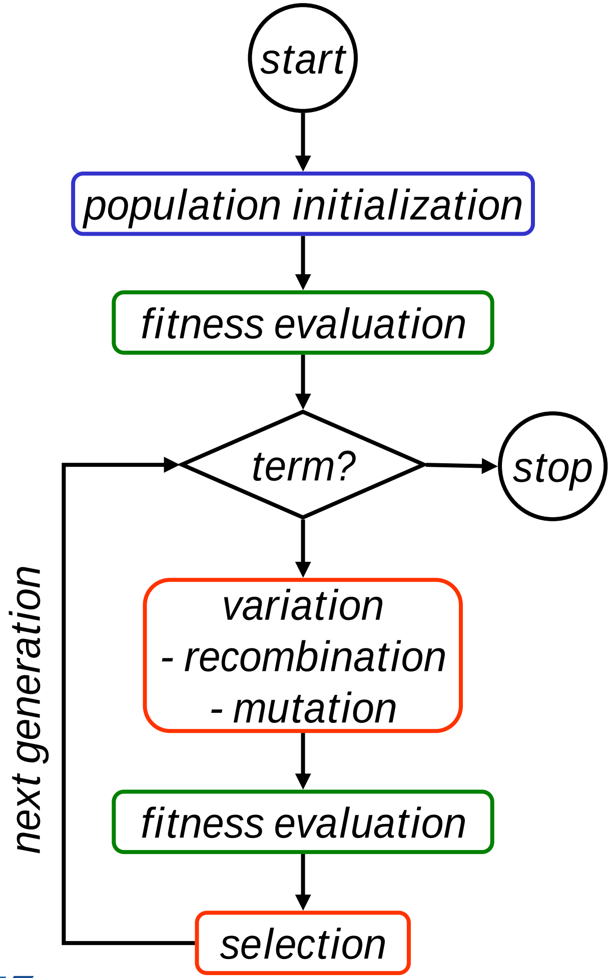
$$\min_{x} \quad c^T x + \sum_{\omega=1}^{\Omega} \pi_\omega Q_\omega(x)$$
$$s.t. \quad Ax \le b,\ x \in X$$

Subproblems: 2nd stage

$$Q_\omega(x) = \min_{y_\omega} \quad q_\omega^T y_\omega$$
$$s.t. \quad W_\omega y_\omega \le h_\omega - T_\omega x,$$
$$y_\omega \in Y$$

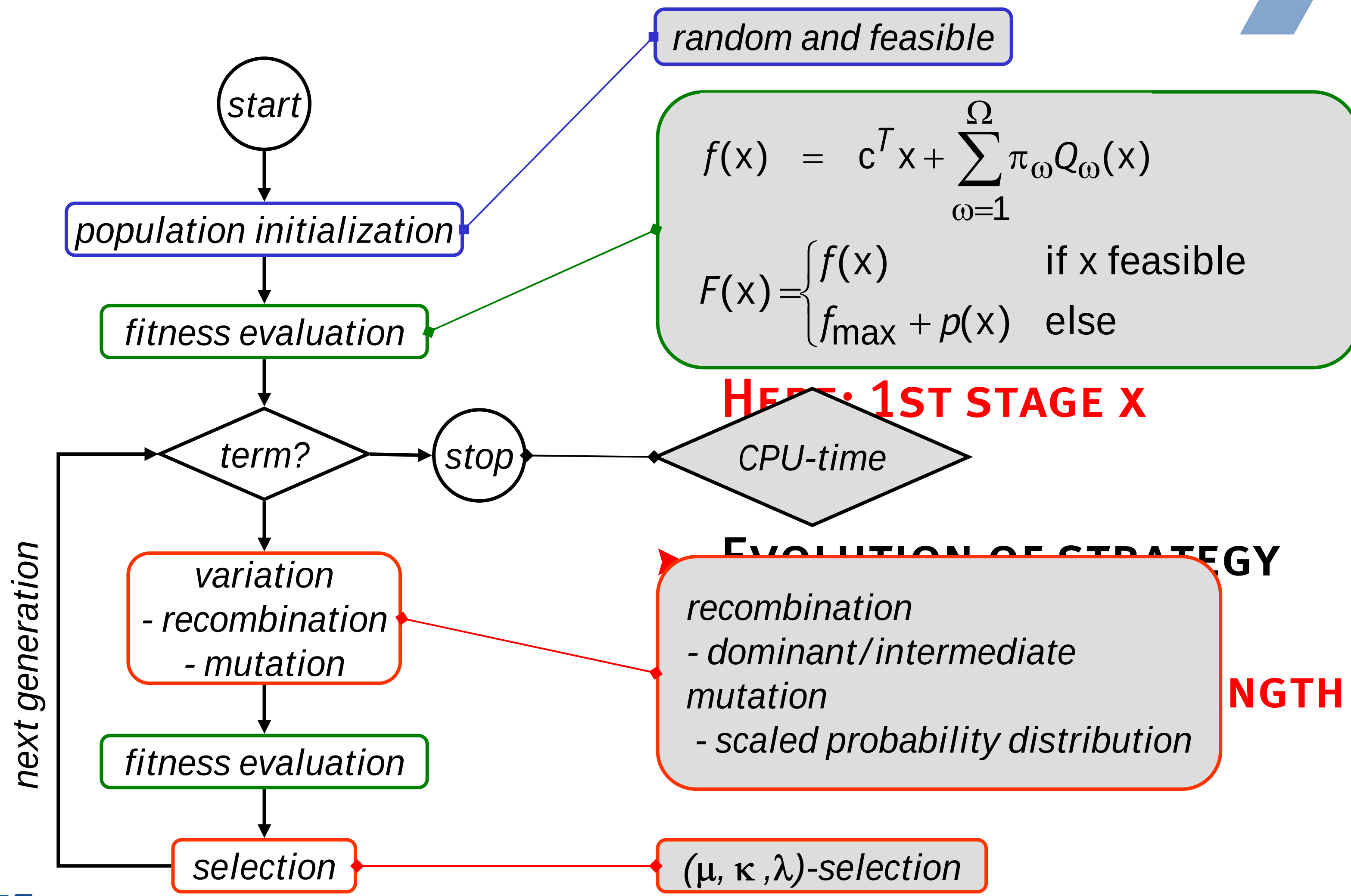
- non-convex in x
- not necessarily feasible (no relative complete recourse)

EVOLUTIONARY ALGORITHMS

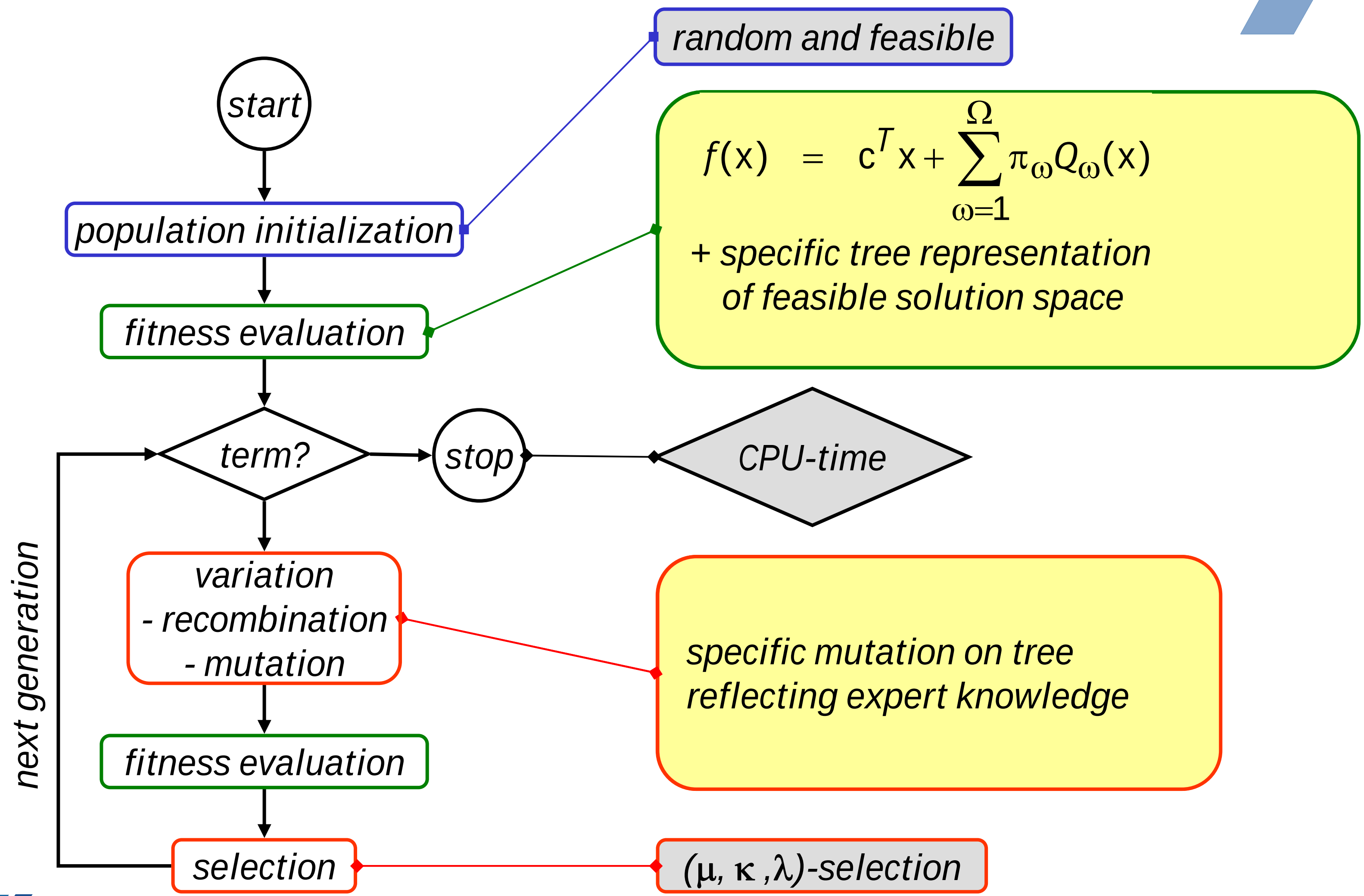


- IMITATE NATURAL EVOLUTION
  "SURVIVAL OF THE FITTEST"
- RANDOMIZED SEARCH
- POPULATION OF INDIVIDUALS
- BLACK-BOX FITNESS FUNCTION
- VARIATION-SELECTION-PARADIGM
  - Variation: diversity
  - Selection: direction
- THEORETICAL PROPERTIES
  - No optimality bounds
  - No convergence guarantee
- CLASSES
  - Genetic algorithms
  - Evolution strategies ...

1. GENERAL EVOLUTION STRATEGY

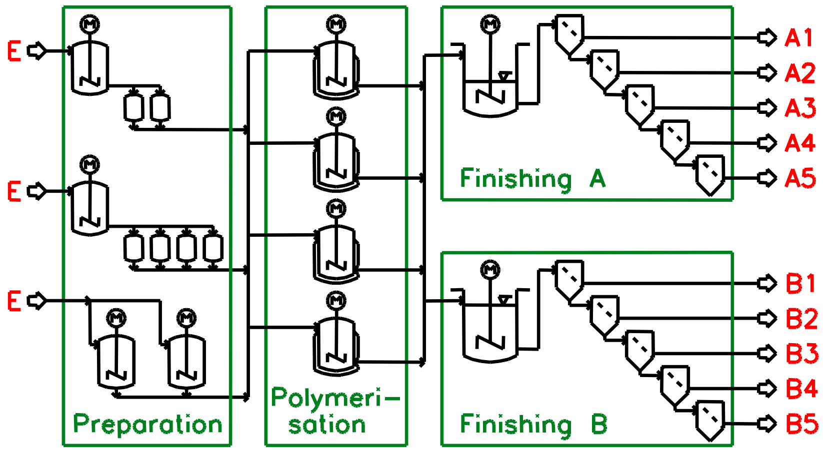


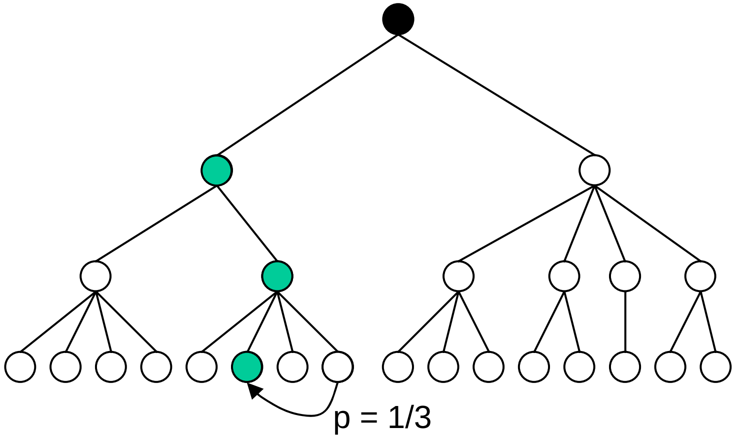
2. Specific Evolutionary Algorithm



SPECIFIC TREE REPRESENTATION

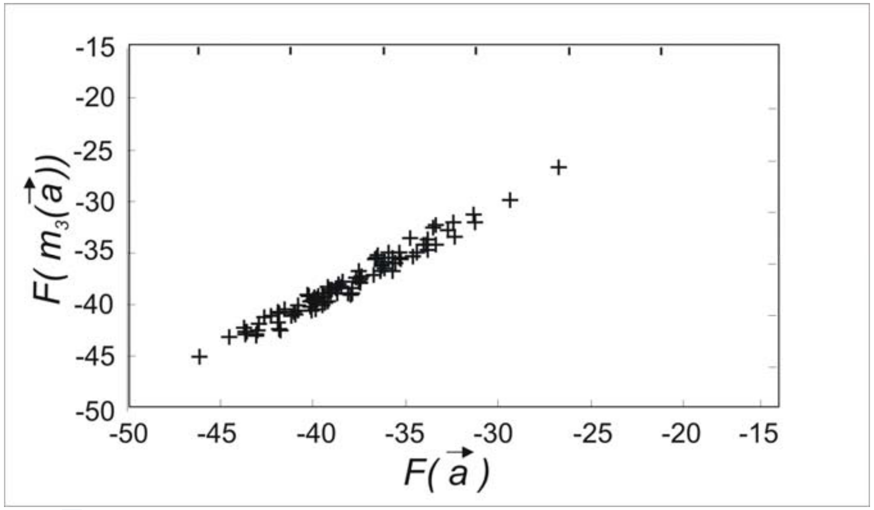
- DECISION TREE OF FEASIBLE SOLUTIONS
- STRONG HIERARCHY OF DECISIONS
  1. Operation *Finishing*
  2. Feed *Finishing*
  3. Number, timing and recipes of batches
- DYNAMIC GENERATION FROM SMALL SET OF SUB-TREES

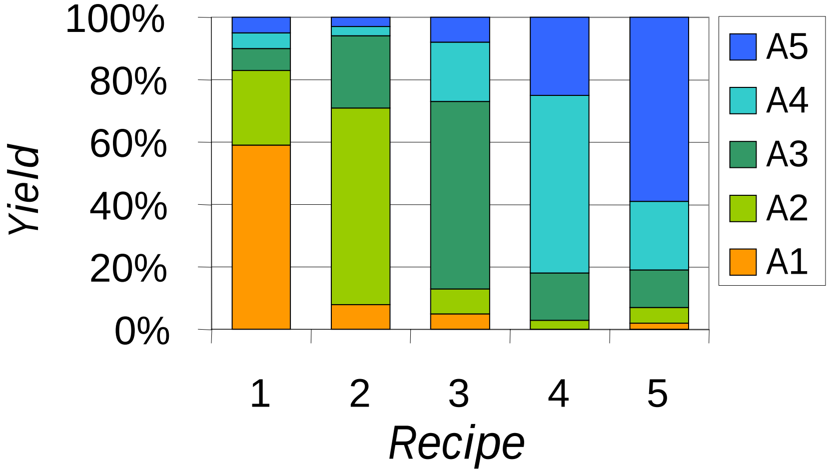




Specific Mutation Operators

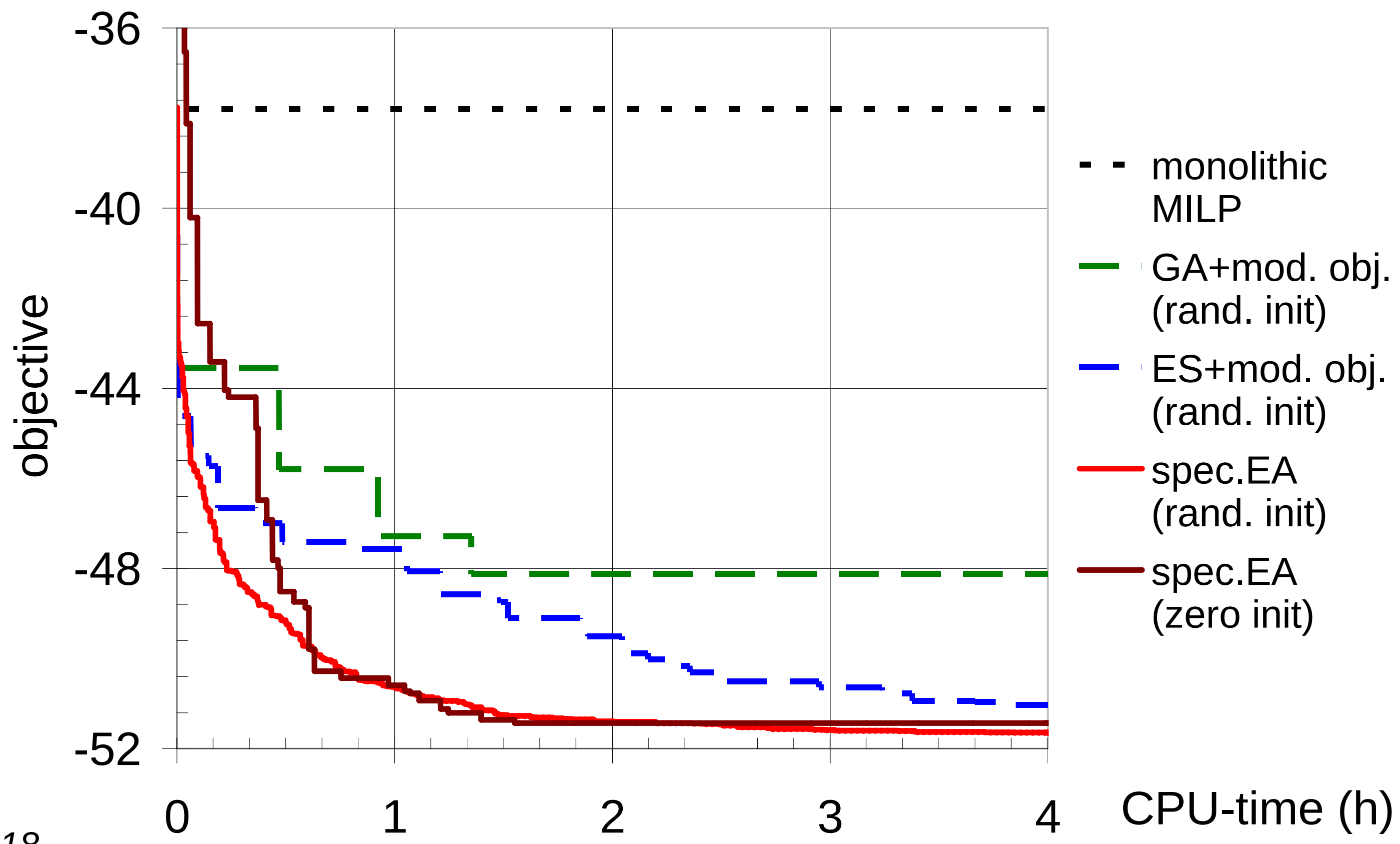
- **Design criteria**
  - Reachability
  - Unbiasdness
  - Scalability
  - Causality
- **Expert knowledge**
  - Similarity of recipes
  - Temporal order





Hybrid Algorithms

- 16 demand scenarios
- 3 first stage intervals
- 4 second stage intervals
- 1,568 discrete variables
- 5,601 continuous variables
- 4,083 constraints

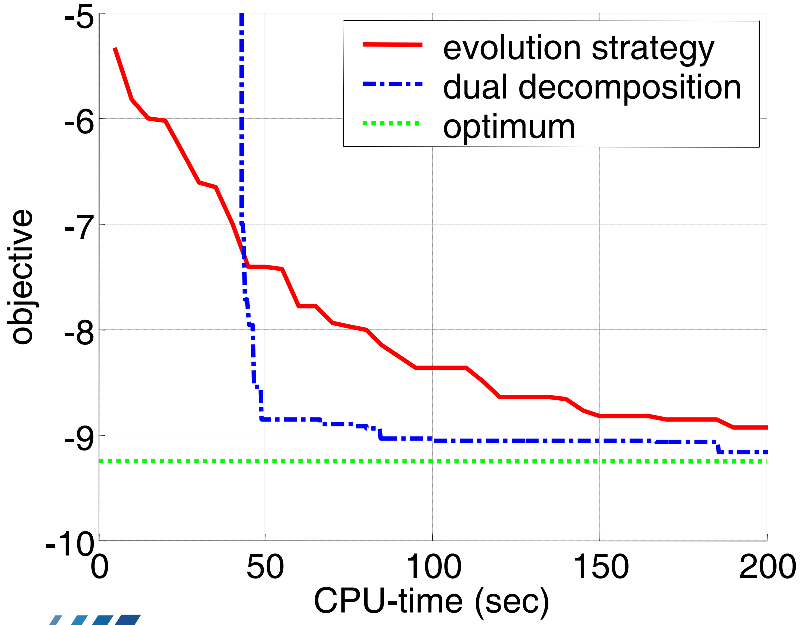


Dual/Scenario Decomposition

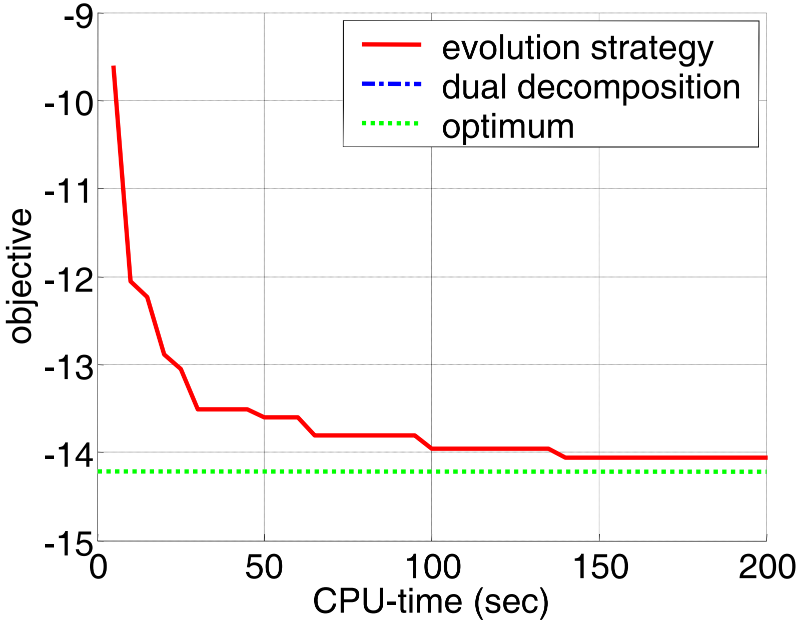
- **Branch & bound-algorithm (*Carøe & Schultz*)**
  1. *Initialization*: Set Z* := ∞ (best current solution) and let *P* (list of untreated problems) consist of the original problem.
  2. *Termination*: If *P* = ∅ then Z* is optimal.
  3. *Node Selection*: Select and delete a problem P ∈ *P* and solve its Lagrangian Dual. If P is infeasible, set $Z^{LD} := \infty$. If $Z^{LD}(P) \geq Z^*$ go to 2.
  4. *Bounding*: Determine heuristically a solution suggestion x^R. If ZR <Z* set $Z^* := Z^R$ and delete all P' ∈ *P* with $Z^{LD}(P') \geq Z^*$.
  5. *Branching*: Select a component $x_{(K)}$ and add two new problems to *P* by extending P by the additional constraints $x_{(K)} \leq x_{(K)}^R$ and $x_{(K)} > x_{(K)}^R$. Go to 3.

Rigorous vs. Stochastic Algorithm

- Uncertain demands
- Relative complete recourse
- 1,144 Variables
- 716 constraints



- Uncertain demands & capacity
- no relative complete recourse
- 1,256 Variables
- 842 constraints



Essence

- Chemical batch scheduling problems as **2-stage stochastic integer programs**
- Fast solution by **structural specific hybrid algorithms**
- Acceleration by systematic **integration of expert knowledge**

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  - cand. math. *Eva Clostermann*, Universität Duisburg-Essen