Uncertainty Analysis for Process Design and Scheduling

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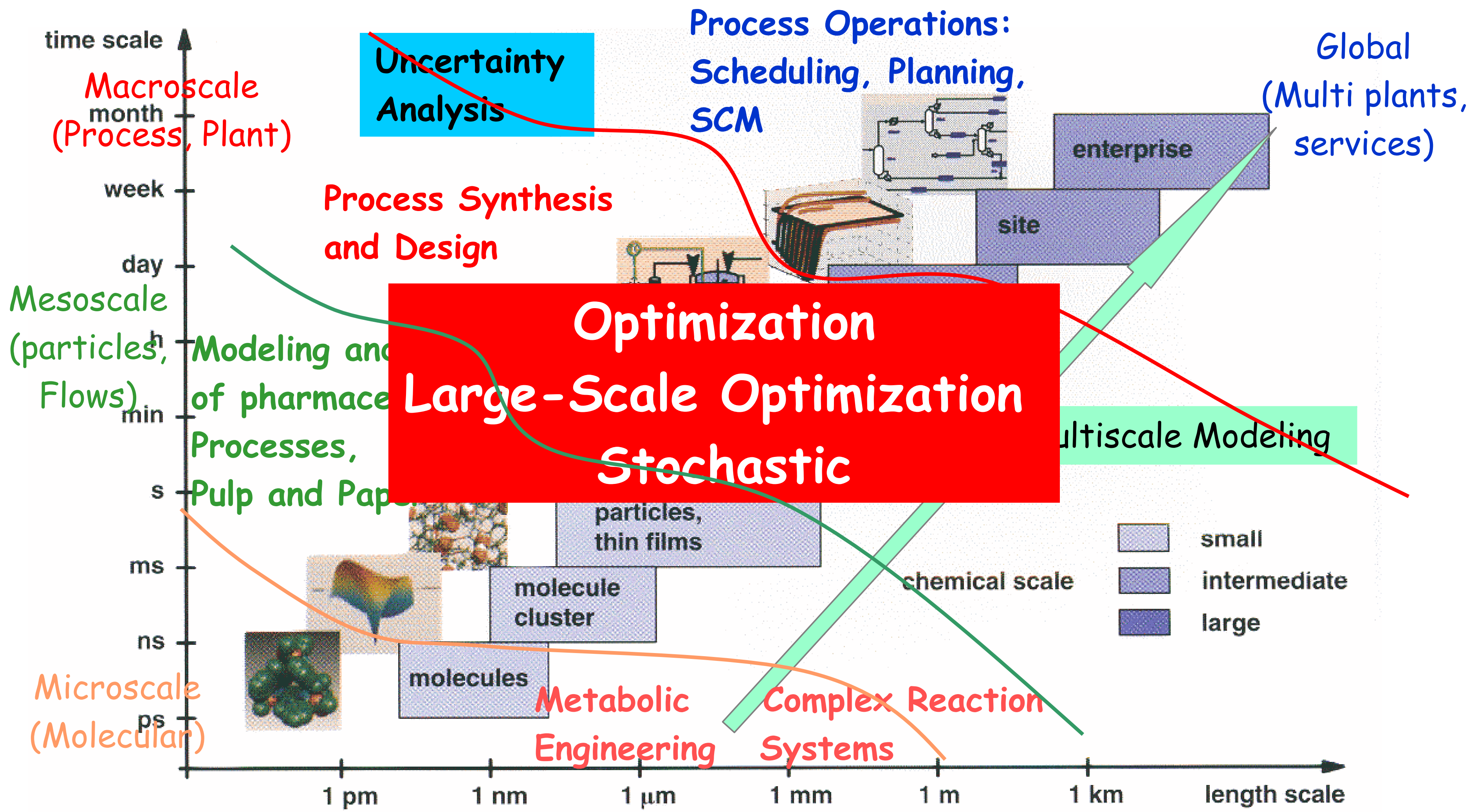
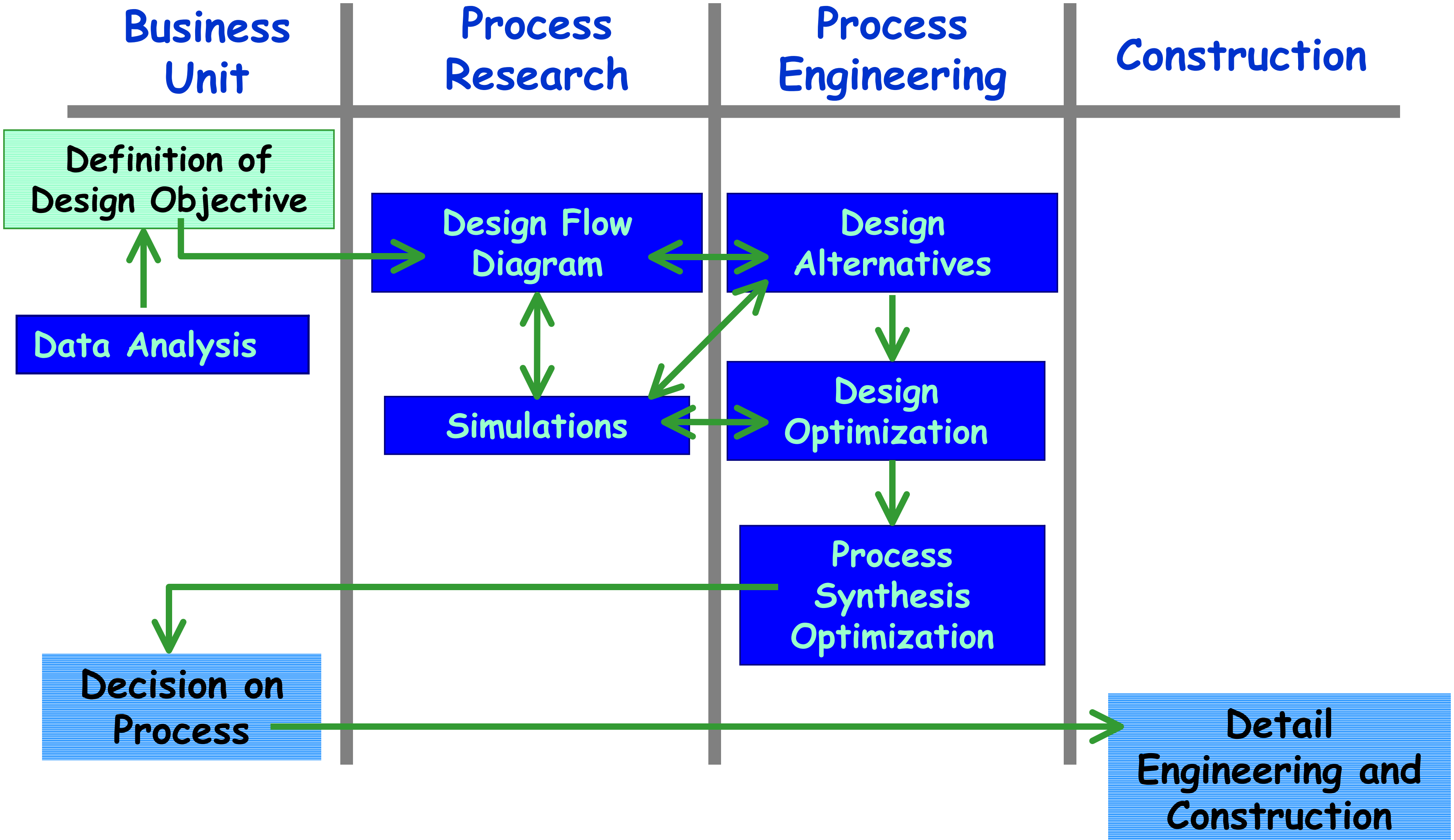
Research Overview of Process Systems Laboratory at Rutgers University



Outline of the Seminar

- Decision-making Process
- Multi-objective Optimization
- Uncertainty Analysis: Measuring the Effects of Uncertainty
- Uncertainty Analysis: Flexibility and Robustness
- Process Synthesis and Design under Uncertainty: Incorporate Demand Description
- Scheduling under Uncertainty
  - Reactive Scheduling
  - Robust Scheduling

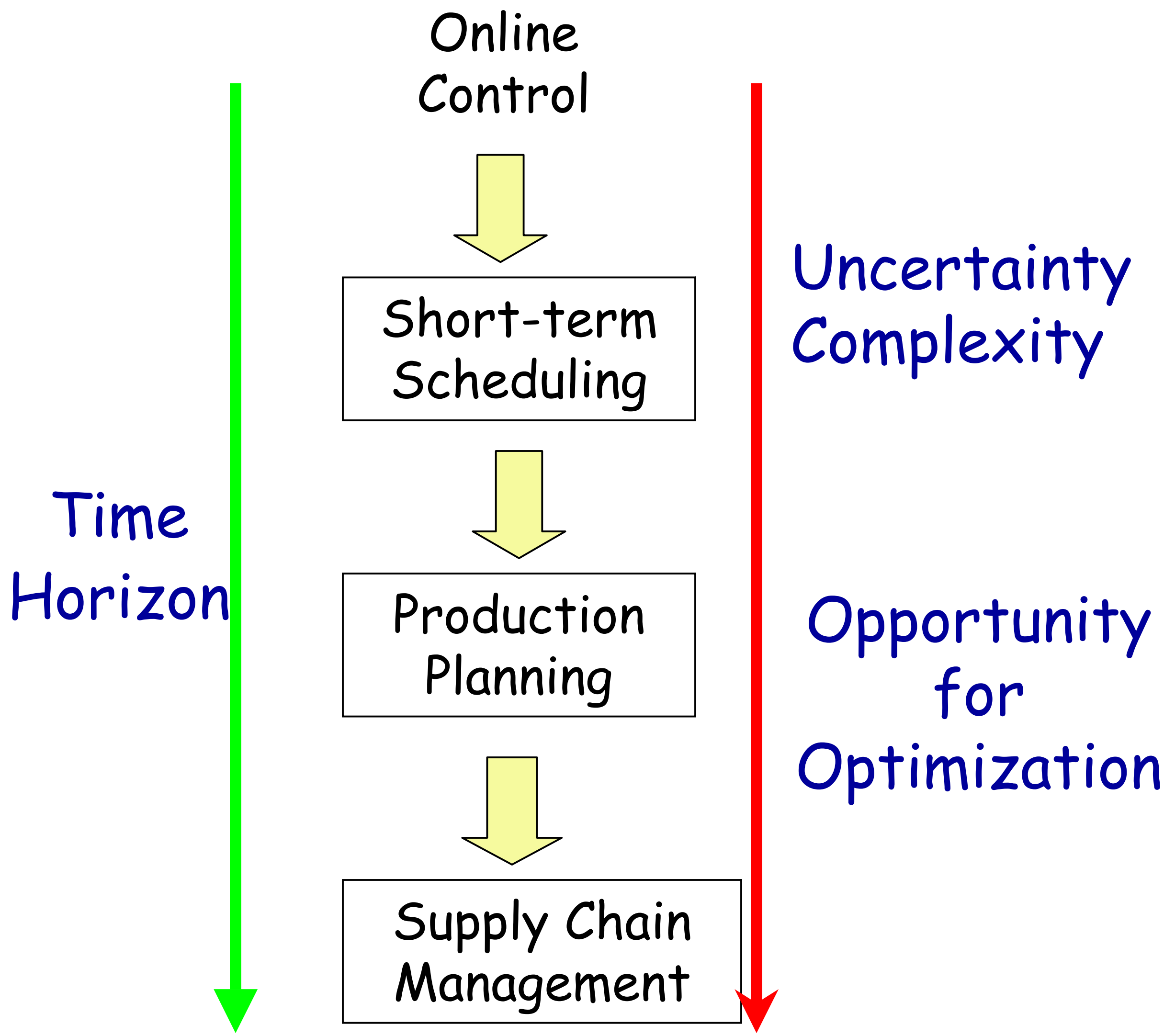
Decision Making:Process Design



Decision Making: Process Operation

Objective

- **Identify and reduce bottlenecks at different levels**
- **Integration of the whole decision-making process**

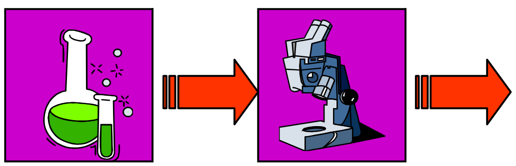


Uncertainty in All Stages of Product Life Cycle

Challenge: Consider Uncertainty at the Early Decision Stage

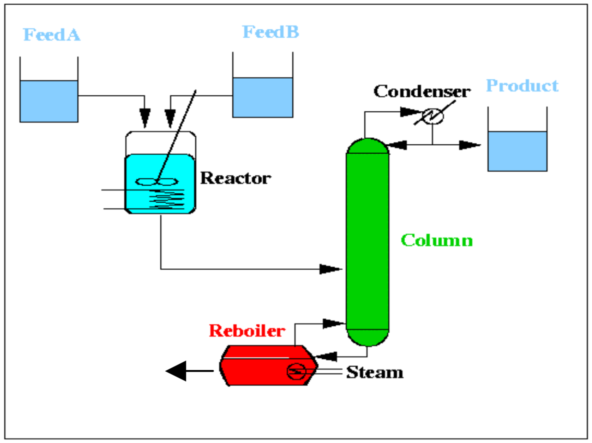
Product Development	Process Design	Process Operations

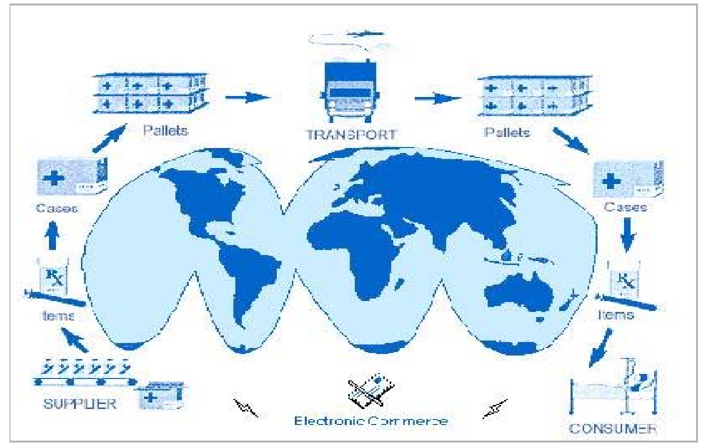
Testing tasks



Probability of Success

0.7	0.4





1 Out of 5000 New Components to the Market

Flexible Manufacturing

Undesirable Production

Flexible-Cost Effective Designs

Infeasible Operation

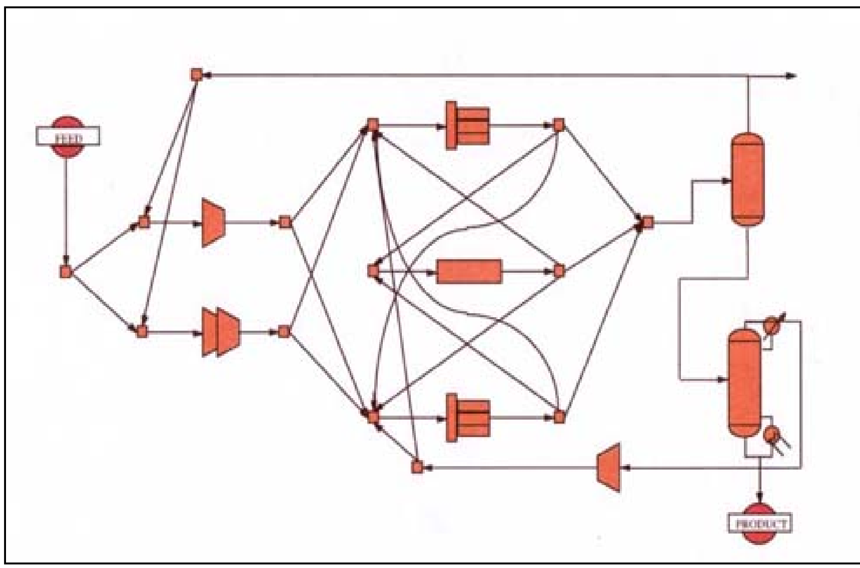
Robust Scheduling
Reactive Scheduling

Feasibility Quantification

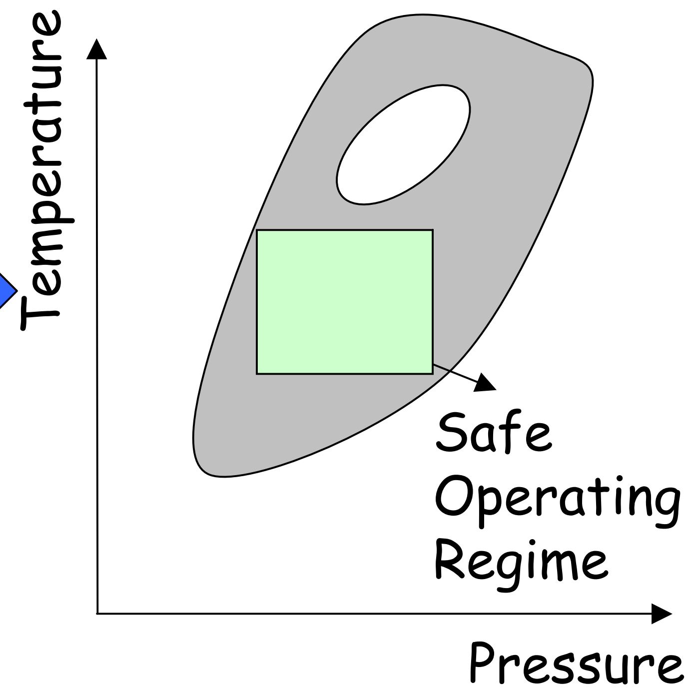
Feasibility Quantification

Given a design/plant or process

Determine the range operating conditions for safe and productive operations



Design

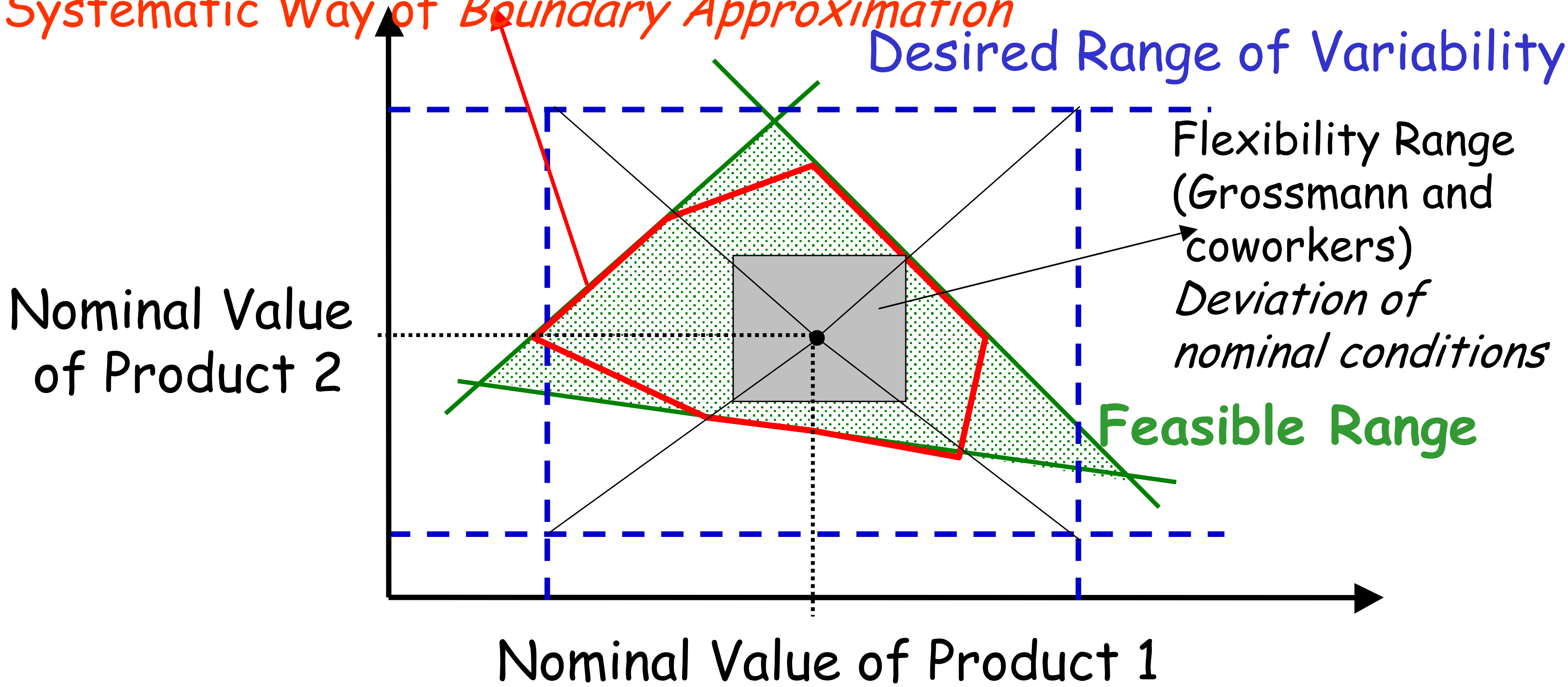


Feasibility Quantification

Convex Hull Approach

(Ierapetritou, *AIChE J.*, **47**, 1407, 2001)

Systematic Way of *Boundary Approximation*



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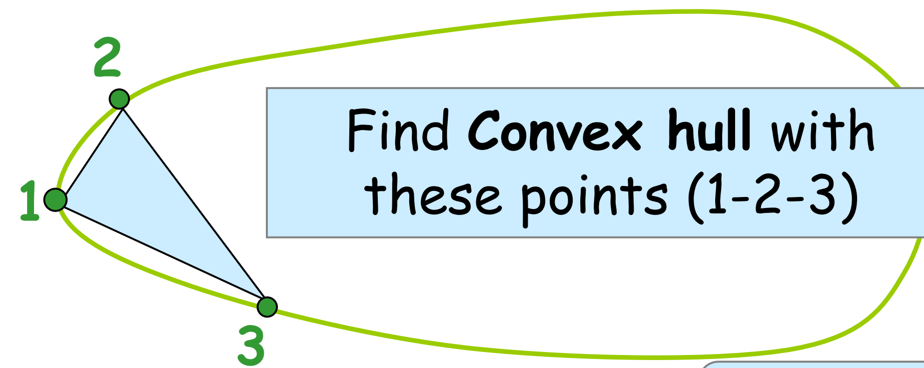
Simplicial Approximation (Inner Hull)

Choose m ≥n+1 points for n dimensions (points 1,2,3)

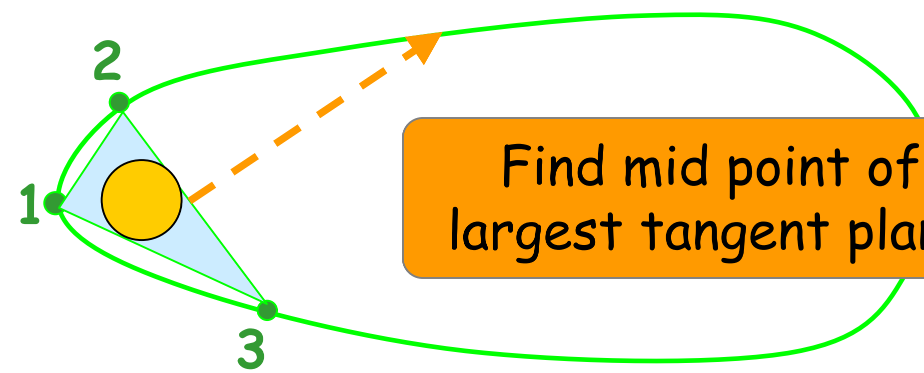


Find **Convex hull** with these points (1-2-3)

Qhull Algorithm

Insert the ***largest*** hypersphere in the convex hull

Solution of one LP

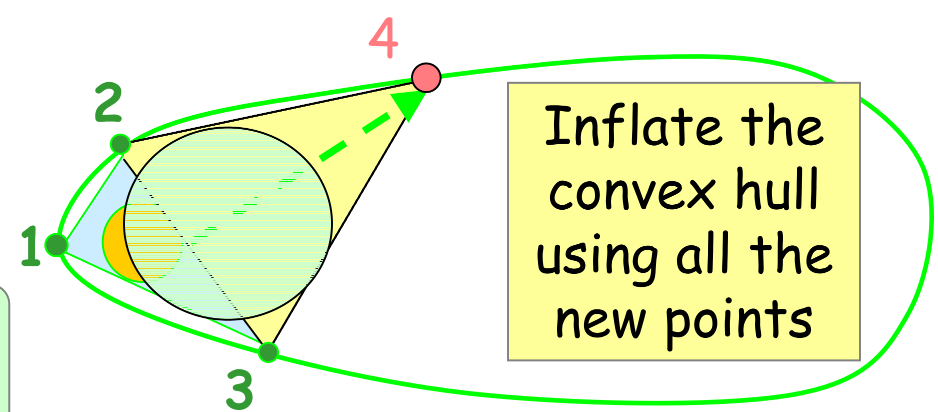


Find mid point of largest tangent plane

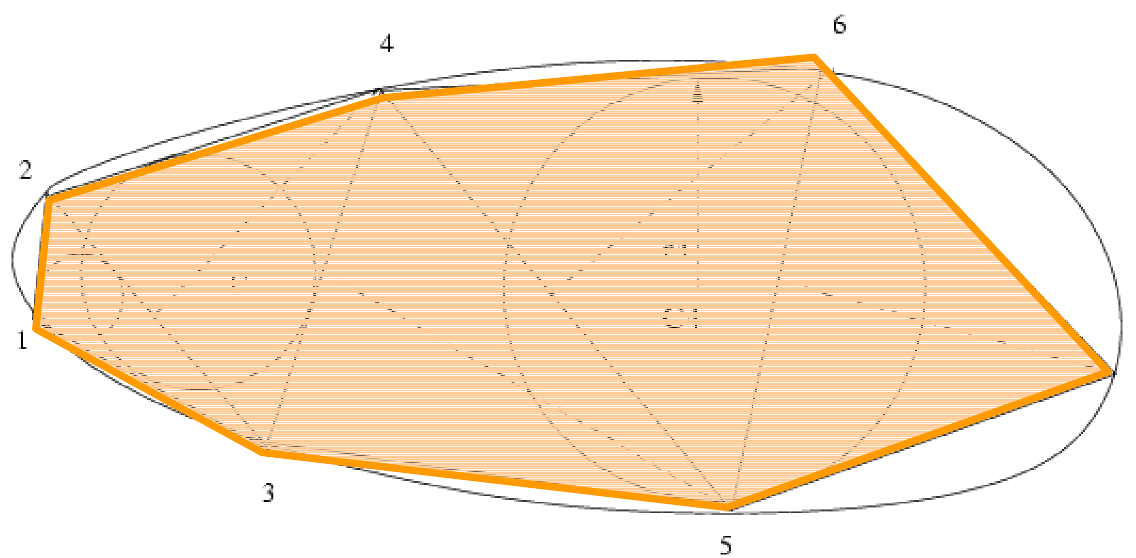
n+1 LPs

Simplicial Approximation (Inner Hull)

Find new boundary points by line search from the mid point



Continue by inserting the ***largest*** hypersphere in the new convex hull



After 4 iterations Approximate Feasible Region1-2-3-4-5-6-7

Simplicial Approximation (Outer Hull)

Obtain initial boundary points by **simplicial approximation**

↓

Determine **tangent hyperplanes** at each boundary point

↓

Points of intersection of the **hyperplanes** are obtained → Find **convex hull** using these points

Overall Feasibility Quantification Approach

Initial set of boundary points (n+1)

One step of the Simplicial approximation: Lower bound of the feasible region

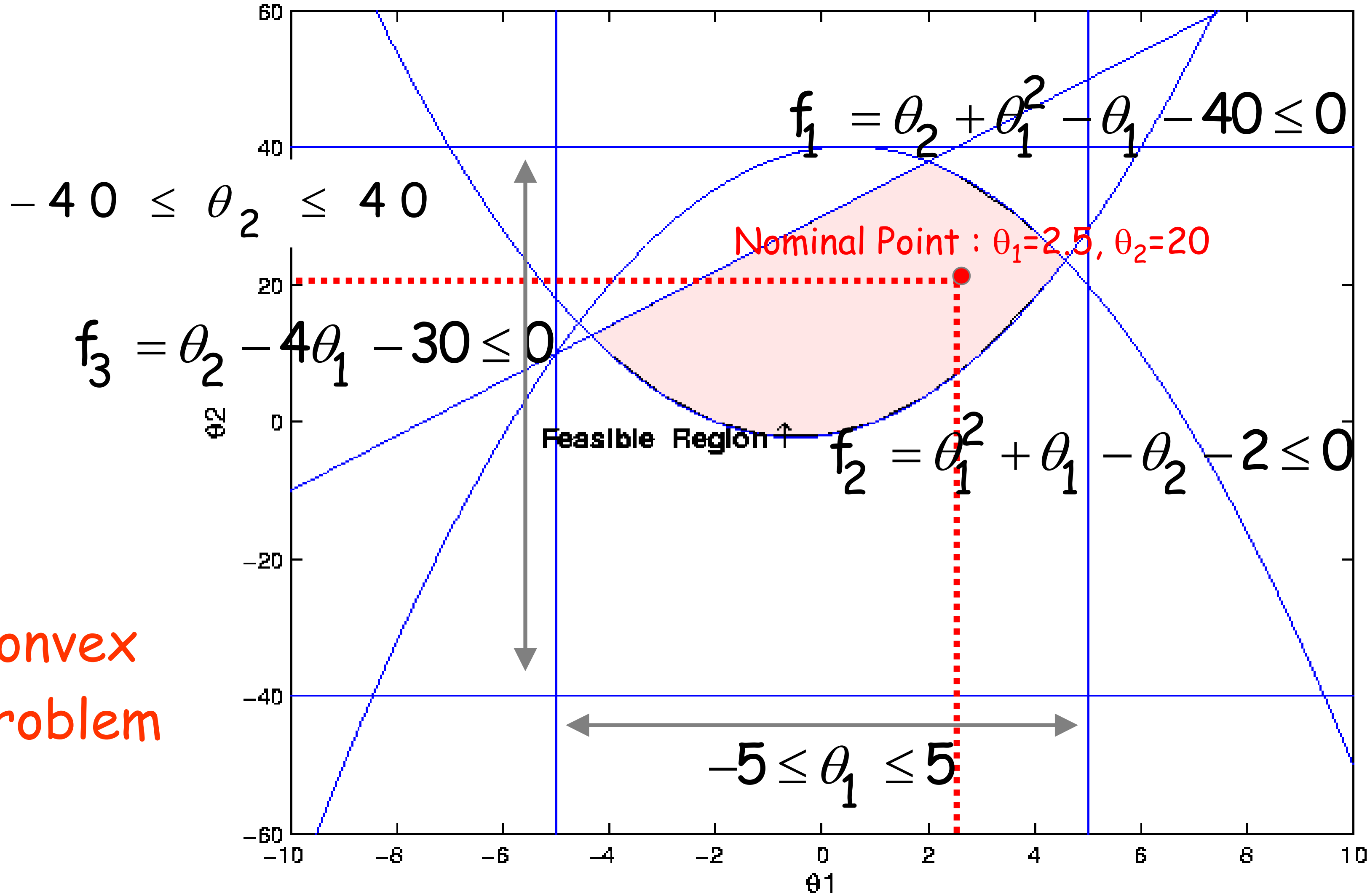
1 NLP

Outer convex hull based on simplicial points: Upper bound

Inflate Convex Hull

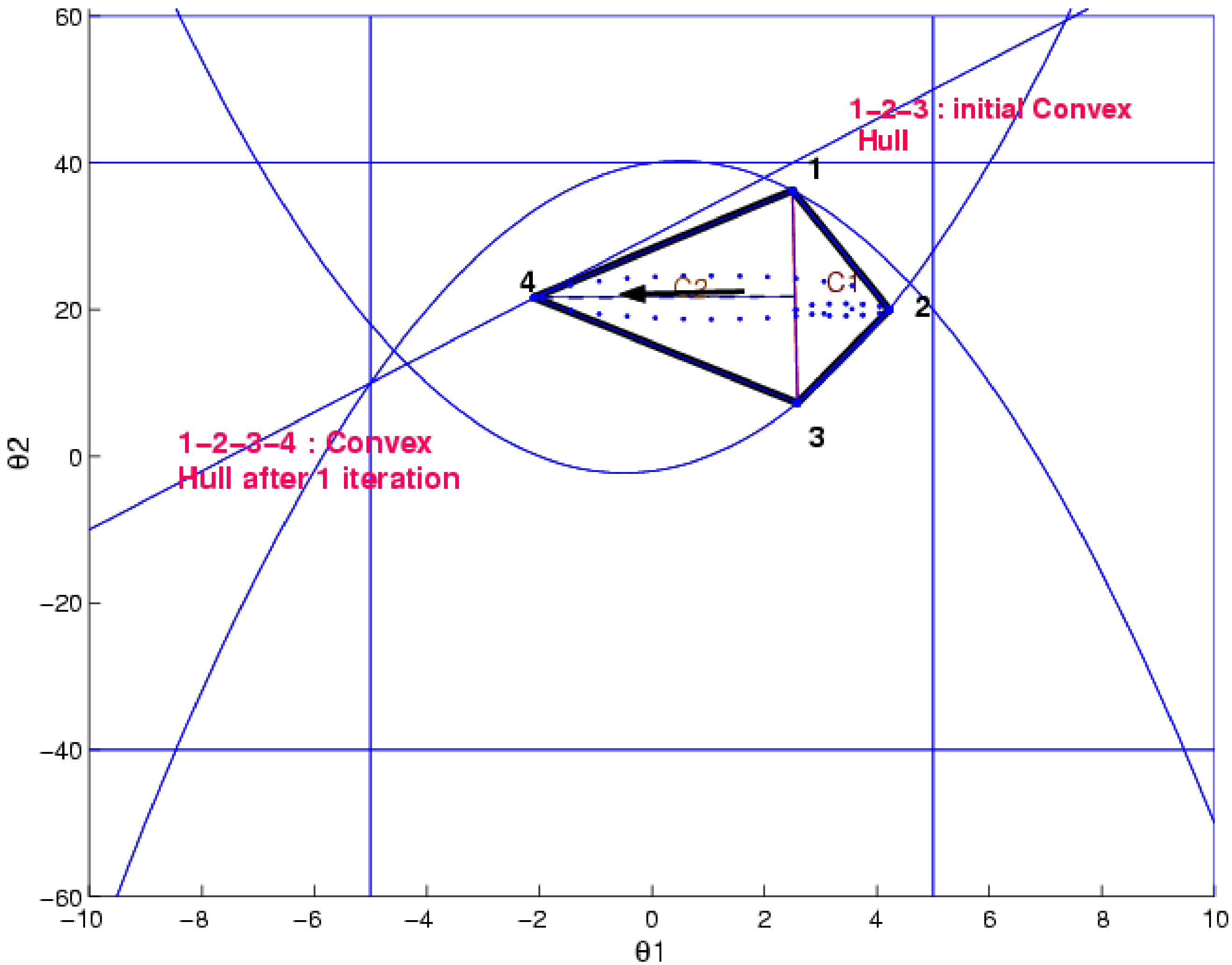
Check convergence UB - LB $< \varepsilon$ or $V^{k+1} - V^{k} < \varepsilon$

Illustrating Problem

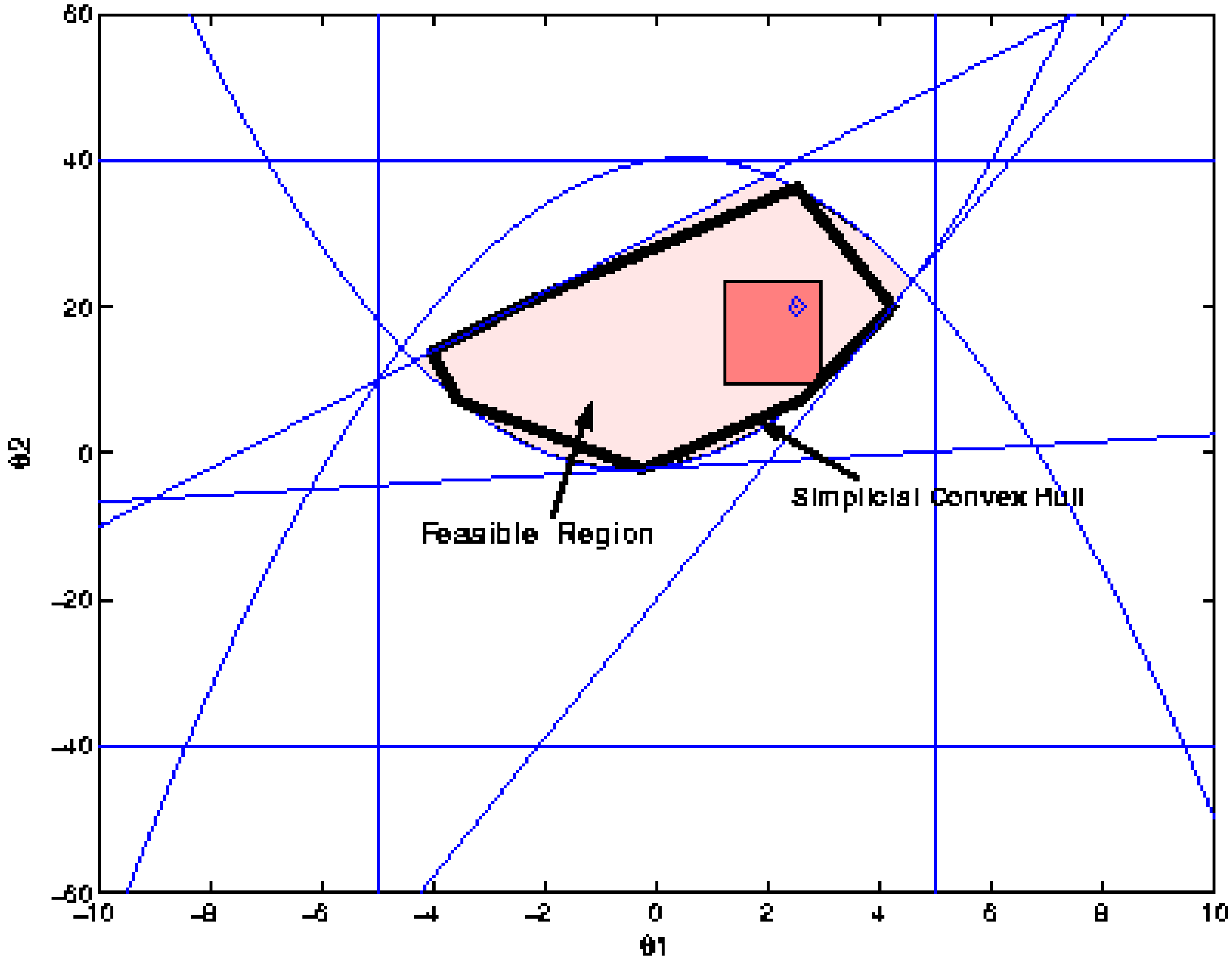


Convex Problem

Illustrating Problem: Simplicial Iterations



Illustrating Problem: Simplicial Convex Hull

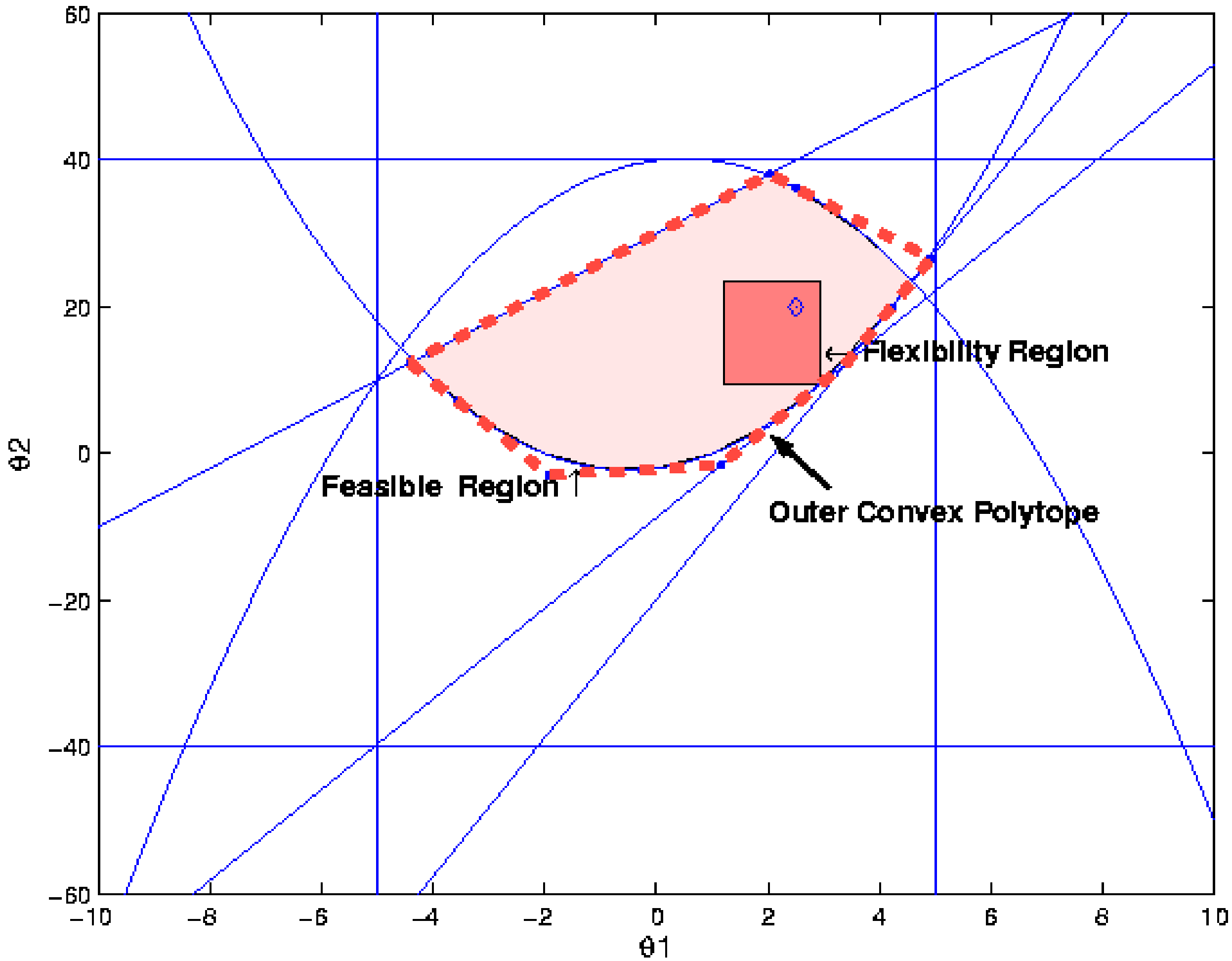


Volume of Simplicial Convex hull: 172.59

Coverage of the actual feasible region: 88.5%

Flexibility Index: 0.174
Coverage of the actual feasible region 14%

Illustrating Problem: Outer Convex Polytope



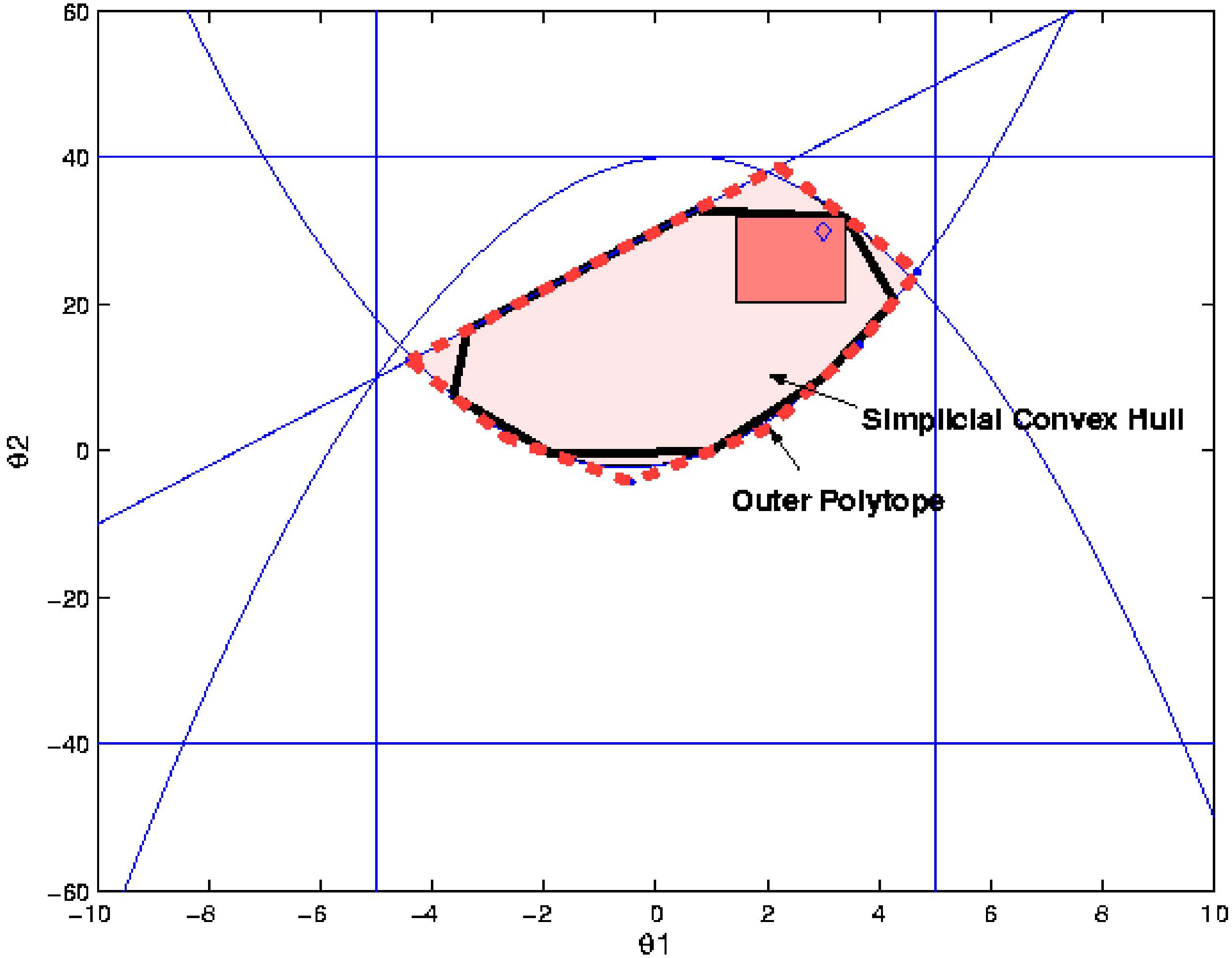
Volume of Simplicial Convex hull: 172.59

Volume of Outer Hull: 209.8 units

Overestimation of the actual feasible region: 7%

SFI: 0.823

Change of Nominal Point $(\theta_1,\theta_2)=(3,30)$



Volume of Simplicial Convex hull: 178.56

Coverage of the actual Feasible region: 91.5%

Volume of Outer Hull: 204.8

Overestimation: 5%

SFI: 0.872
(Difference ~5.6%)
Independent of Nominal point

Flexibility Index: 0.095
(Difference ~45%)
Nominal point dependent

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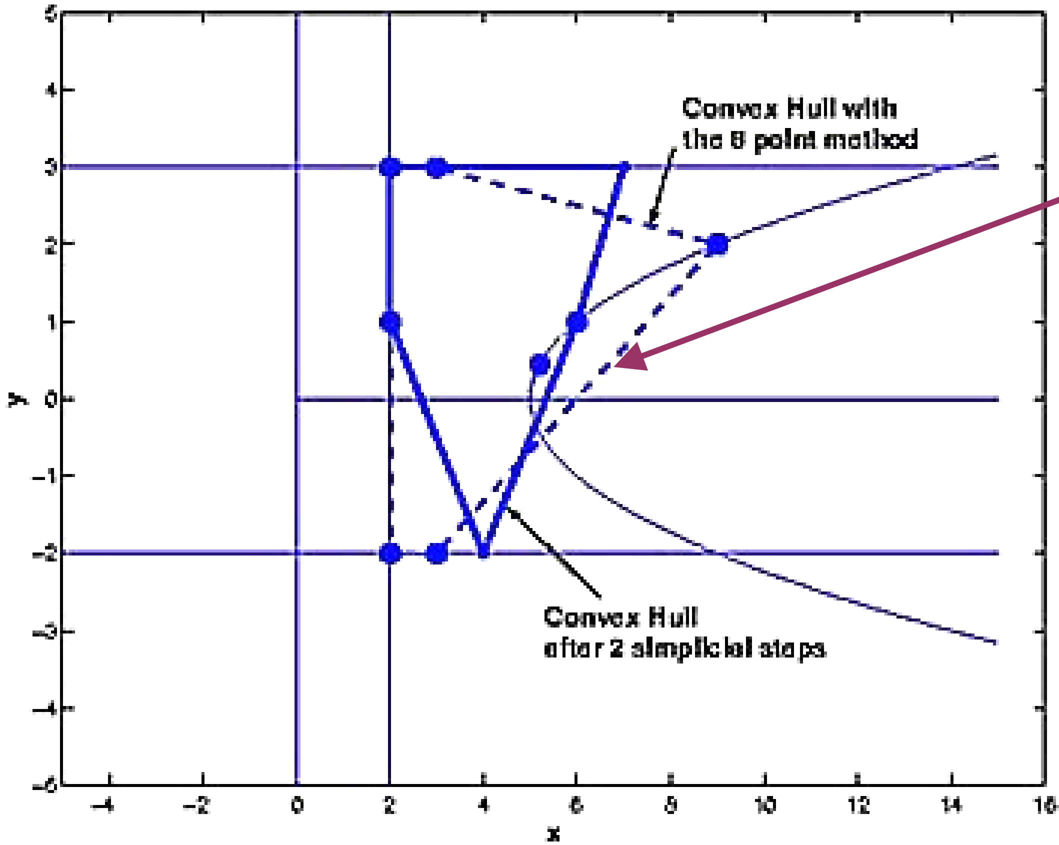
Noncovex Problems: Need for Alternative Methods



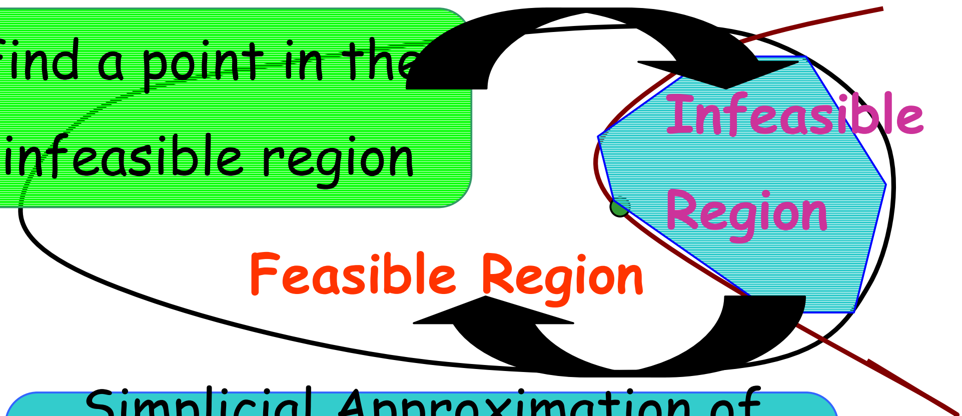
Failure of Existing Methods due to Convexity Assumptions

Assumption: The Non-Convex Constraints can be identified a priori

Proposed Approach: Non-Convex Regions

Select a constraint from the set of nonconvex constraints, NC

Find a point in the infeasible region

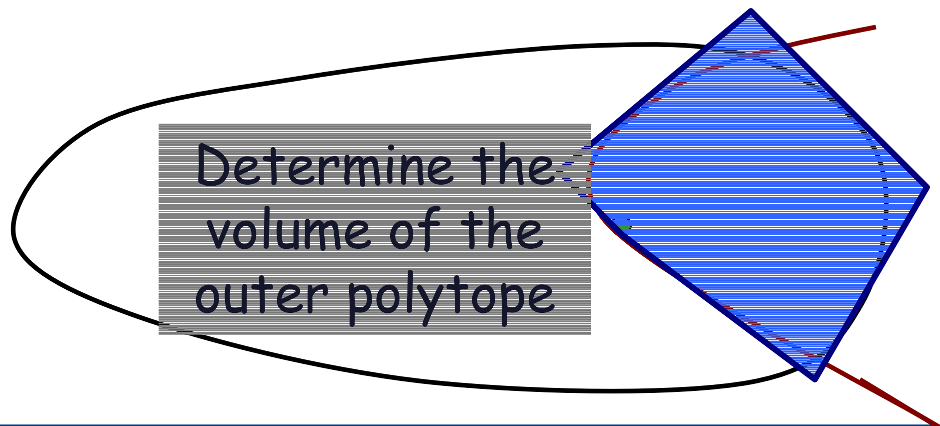


Simplicial Approximation of the Infeasible Region

Modified Feasibility Problem (NLP)

Develop the Outer Polytope for the Simplicial Region

Determine the volume of the outer polytope



Proposed Approach: Non-Convex Regions

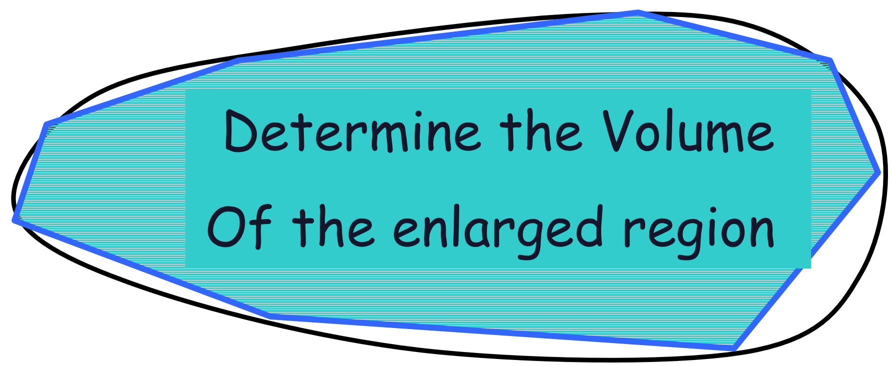
Is NC Empty

NO

Choose another non-convex constraint and continue

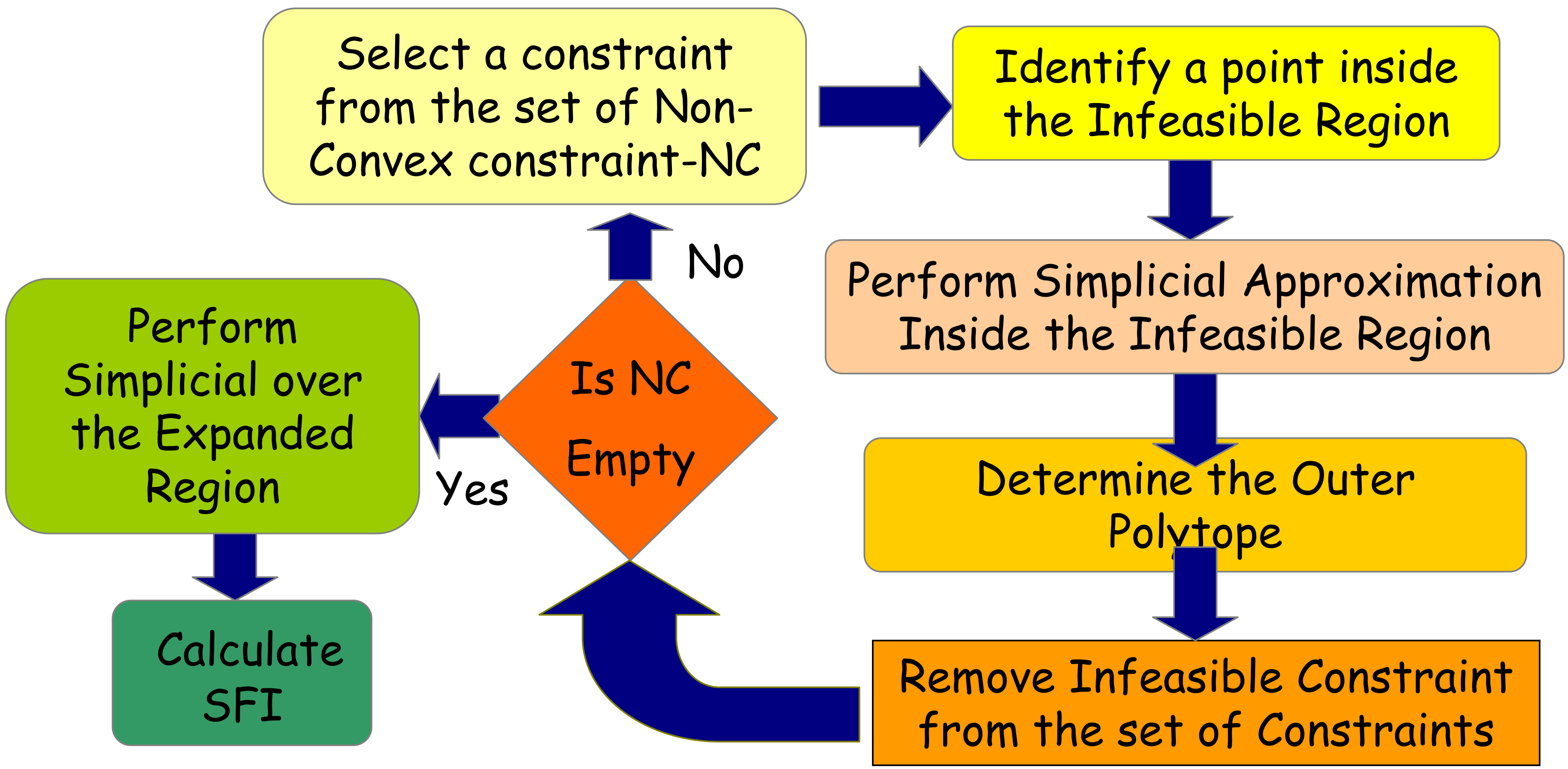
YES

Remove the non convex constraints and perform Simplicial Approximation over the enlarged region

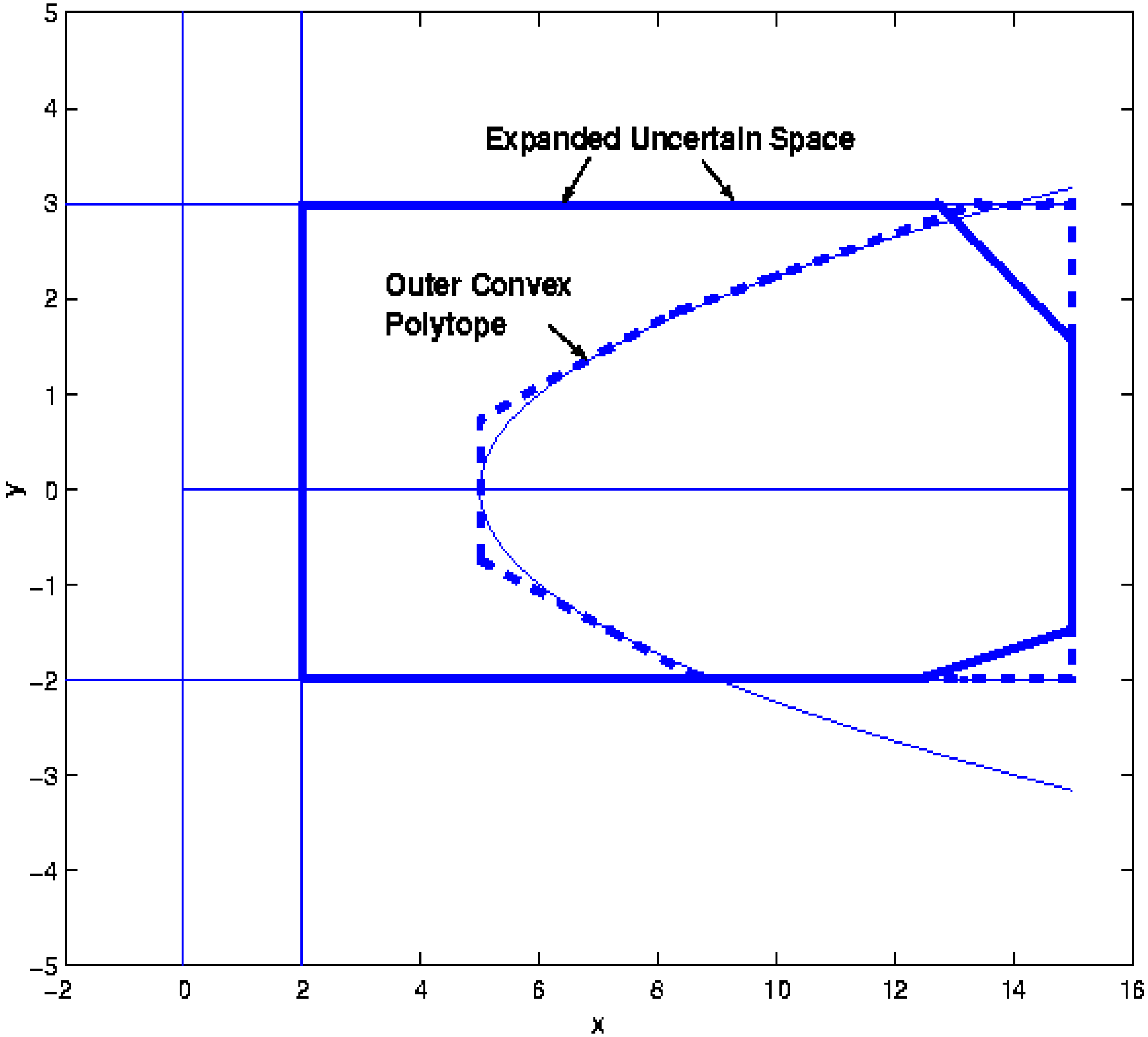


$$\text{SFI} = \frac{\textit{Volume of expanded convex hull} - \sum \textit{Volume of infeasible convex polytopes}}{\textit{Volume of the expanded convex hull}}$$

Approximation of Non-Convex Regions



Illustrating Example



Volume of Expanded Convex hull = **62.66**

Volume of Infeasible Regions = **39.13**

SFI : 0.386 (3.5%)

$$f_1 = 2 - x \le 0$$

$$f_2 = -y - 2 \le 0$$

$$f_3 = y - 3 \le 0$$

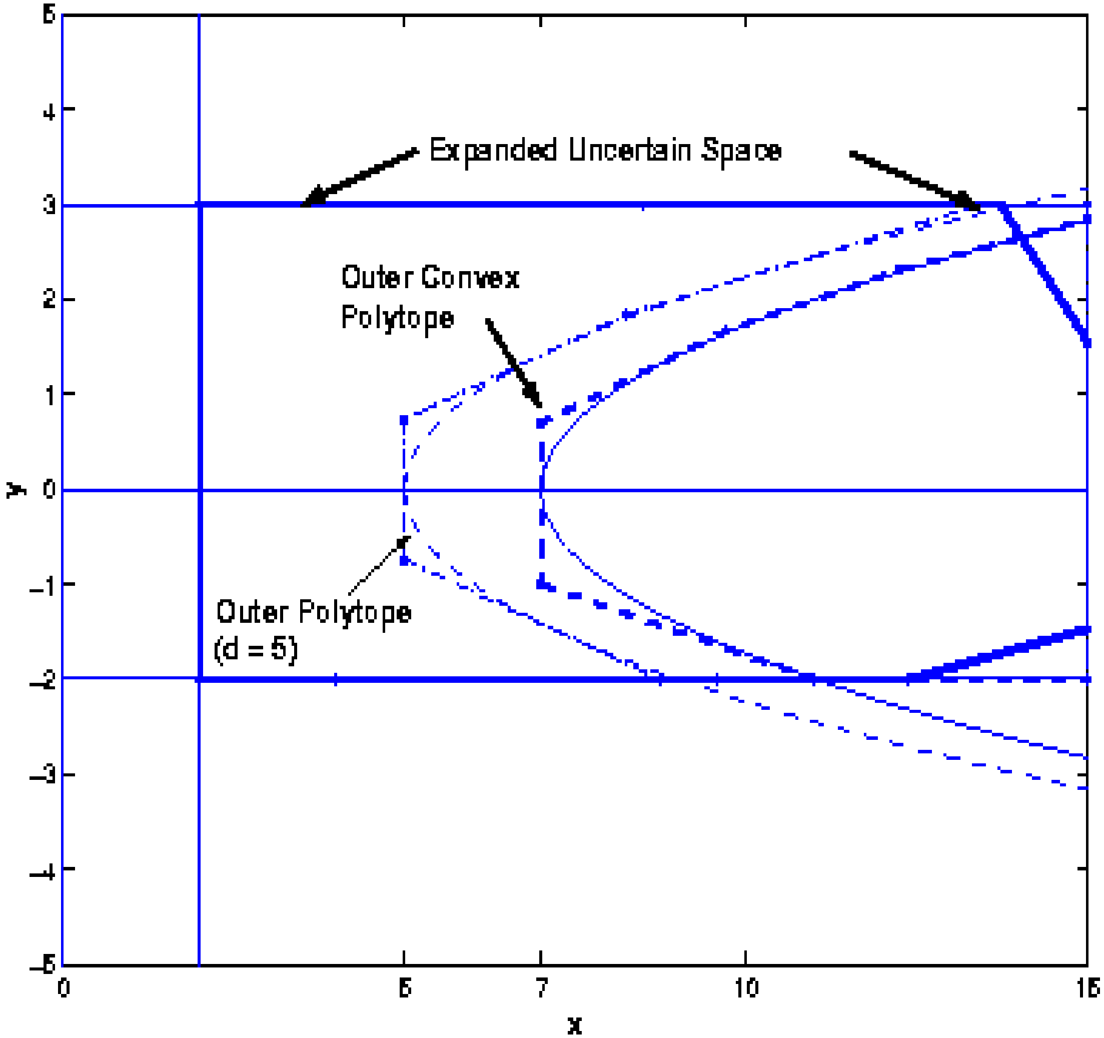
$$f_4 = x - d - y^2 \le 0$$

$$d = 5$$

$$2 \le x \le 15$$

$$-2 \le y \le 3$$

Illustrating Example: Relevance of SFI



Volume of Expanded Convex hull = **62.66**

Volume of Infeasible Regions = **29.4**

d = 7 SFI : 0.54

d = 5 SFI : 0.386

SFI correctly predicts the increased flexibility of the new design

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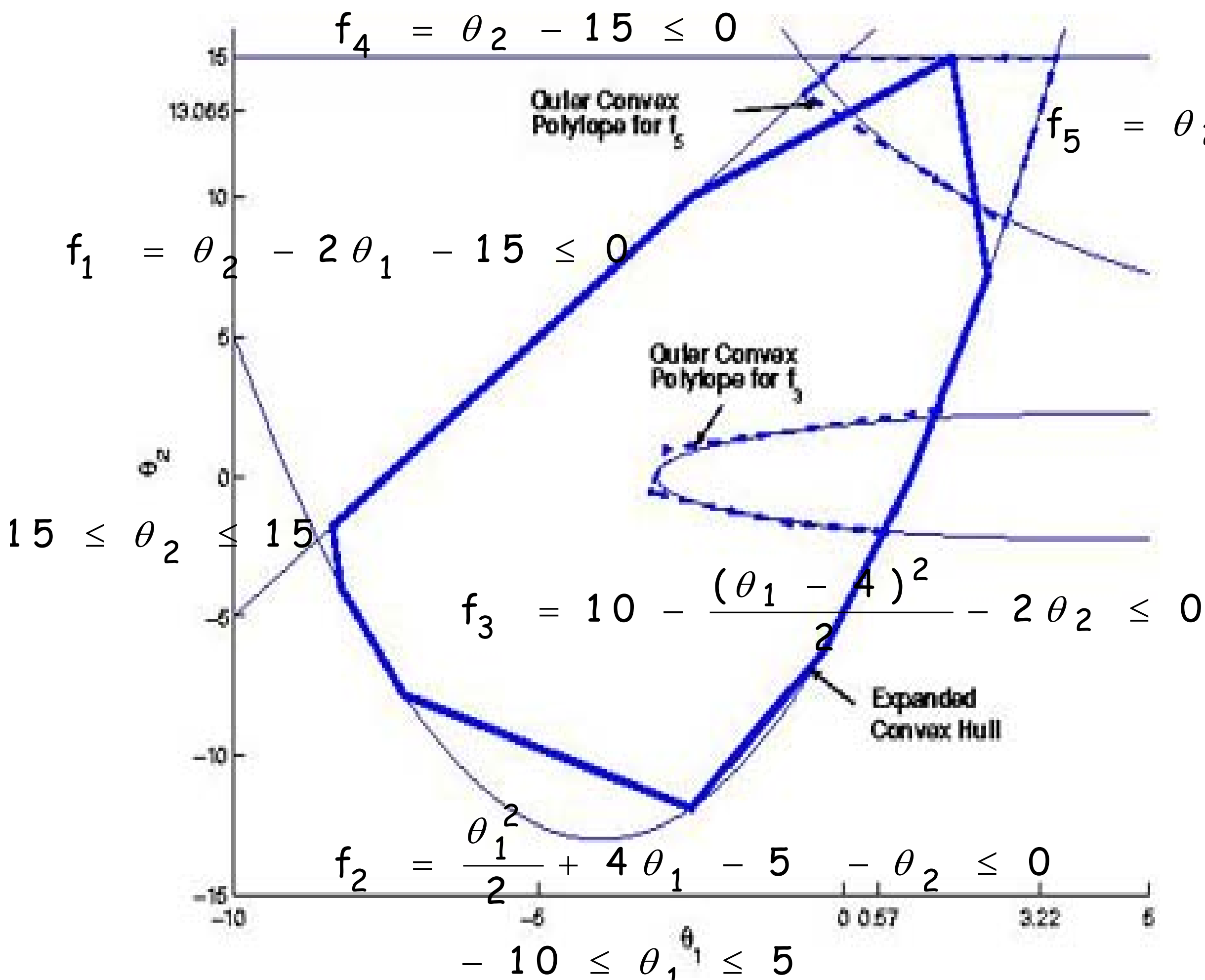
Multiple Non-Convex Constraints



Volume of Expanded Convex hull = **156.7**

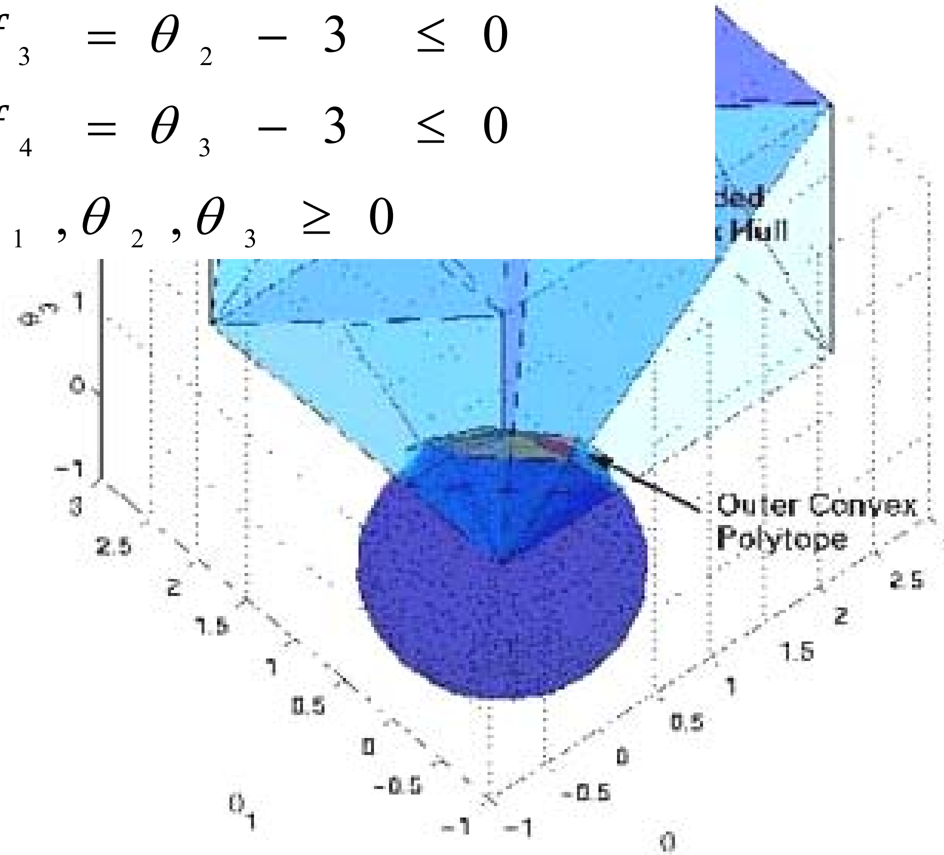
Volume of Infeasible Regions =

12.9 + 14.1 = 27.0

SFI : 0.83 (1.5%)

Multi-Parametric Case

$$f_1 = \theta_1^2 + \theta_2^2 + \theta_3^2 \geq 1$$
$$f_2 = \theta_1 - 3 \leq 0$$
$$f_3 = \theta_2 - 3 \leq 0$$
$$f_4 = \theta_3 - 3 \leq 0$$
$$\theta_1, \theta_2, \theta_3 \geq 0$$



Volume of Expanded Convex hull = **26.5**

Volume of Infeasible Regions = **0.978**

<u>SFI</u> : 0.978 (0.2%)

<u>Computational Complexity</u>

NLP (**Line search**)

Illustrating Example := **18**

3 Uncertain parameters := **21**

Computational Complexity

- **Simplicial Approximation Approach:**
  k iterations: k line searches

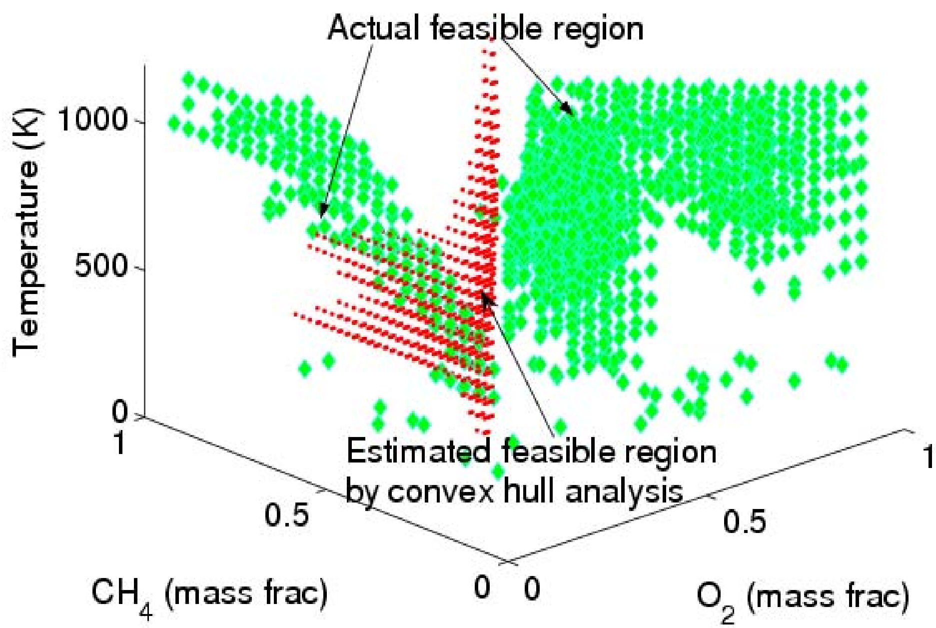
- **Outer Polytope Generation:**
  O(n) process

- **QuickHull Algorithm: (Convex Hull)**
  $O(n \log r)$ $n \leq 3$ and $O(nf_r/r)$ for $n \geq 4$

  n = size of input with r *processed points and* f_r *is the maximum number of facets for* r *vertices*

Limitations

Feasible region of reduced methane mechanism



Feasible region can be highly nonconvex, sometimes disjoint

Conventional feasibility analysis techniques do not perform adequately

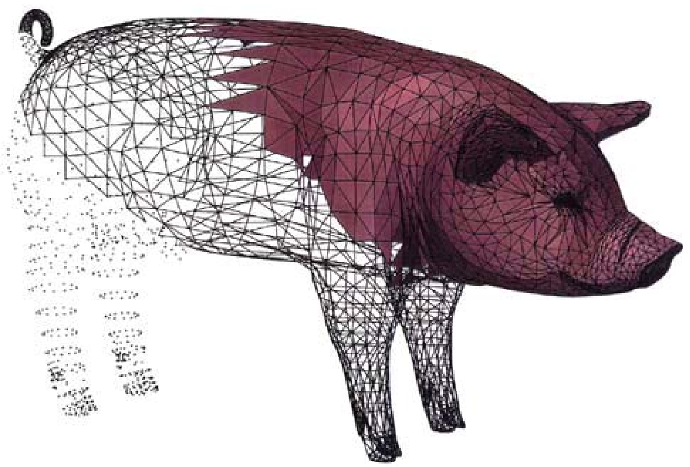
Convex hull analysis cannot capture the disjoint region
Can over-predict the feasible region

New technique for accurate estimation of nonconvex and disjoint feasible regions

Surface Reconstruction Ideas

Problem definition of surface reconstruction:

Given a set of sample points, determine the shape formed by these points



- Identify points constituting the boundary of the data set
- Join boundary points to reconstruct the surface

Analogous to problem of feasibility analysis

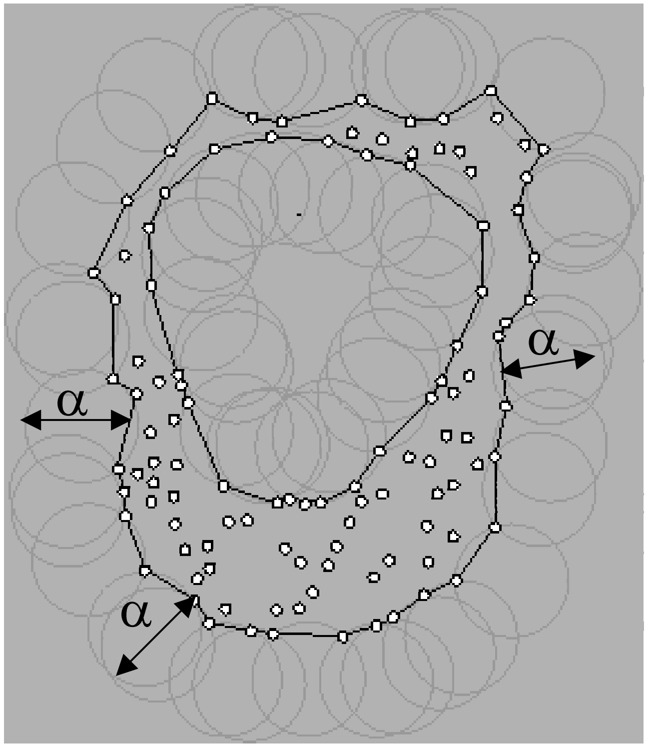
Determine mathematical representation of the boundary of the feasible region

Improved Feasibility Analysis by $\alpha-$shapes

Given a set of points, determine the shape formed by these points

Eliminate maximum possible circles of radius α without eliminating any data point

H. Edelsbrunner, 1983

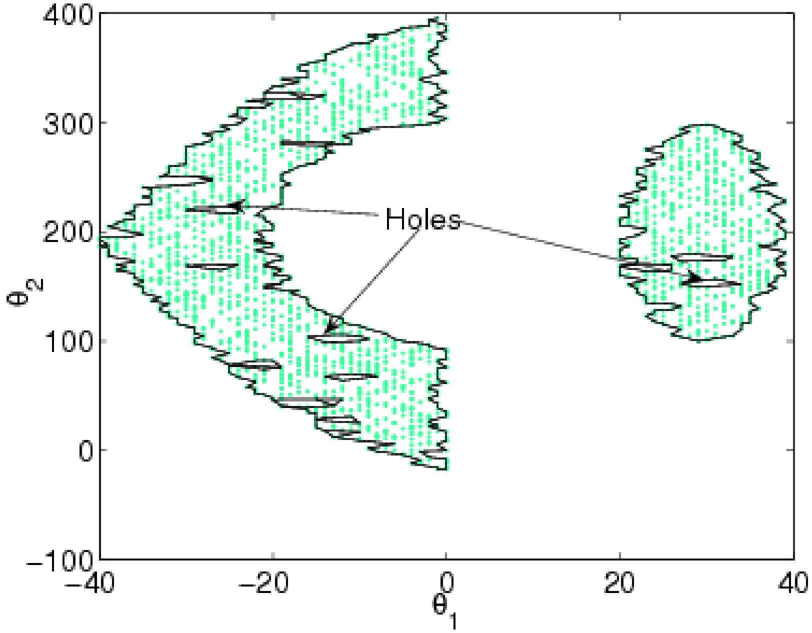


For $\alpha \to 0$ the α shape degenerates to the original point set

For $\alpha \to \infty$ the α shape is the convex hull of the original point set

(Ken Clarkson http://bell-labs.com/netlib/voronoi/hull.html)

Selection of α value for $\alpha-$shapes



Value of α controls the level of details of the constructed surface.

α is a function of sample size (n)

α is a function of inter-point distance

Determination of α value

Mandal& Murty, 1997

Construct minimum spanning tree (MST) of sampled data points

Evaluate $\mathcal{L}_n$ = sum of Euclidean distance between points of the MST

$$\alpha \text{ value} = \sqrt{\frac{\mathcal{L}_n}{n}}$$

Algorithm for Feasibility Analysis

Sample the feasible space

Construct MST of sampled data to determine α value

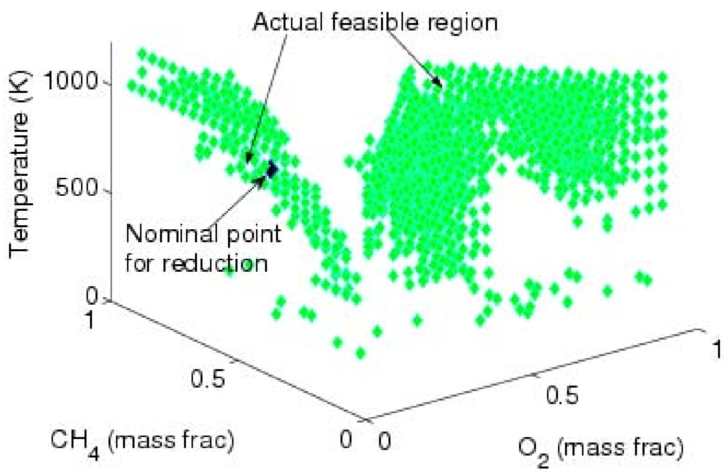
Construct an α shape of sampled data points

Points constituting the boundary of the feasible region

Join points by a line in 2-d, by triangle in 3d

Obtain polygonal representation of the feasible region

Sampling Technique



Implementation of this idea requires sampling of the feasible region

Common sampling techniques sample the parameter space based on the distribution of the uncertain parameter

Typically, the feasible region constitutes a small fraction of the entire parameter space

Uniform sampling of entire parameter space can be expensive

Require new technique which samples the feasible region with minimum total function evaluations

Reformulation of Sampling Problem

Obtain good sample of feasible region with less function evaluations

Sampling problem framed as an optimization problem

$$\max_{\theta} \quad V_{feas}$$

$$\text{subject to: } \left(f_1\right)_\theta \le 0$$
$$\left(f_2\right)_\theta \le 0$$
$$\vdots$$
$$\left(f_n\right)_\theta \le 0$$

θ: sampled parameter value

Objective function V_{feas} (volume of the feasible region) evaluated by constructing the α-shape using the sample points

Improved only when the sampled point is feasible

Formulated optimization problem is solved using Genetic Algorithm

GA has the inherent property of concentrating around good solutions

Sampling Technique using GA

$$\underbrace{0\;1\;1}_{V_1}\;\underbrace{0\;1\;0\;0}_{V_2}\;\underbrace{1\;1}_{V_3}$$

chromosome

Optimization variables encoded as a string of bits

Strings are appended to form a chromosome

Solution procedure starts with a population of chromosome

Population of chromosome evolve through :
- **Reproduction**
- **Crossover**
- **Mutation**

Reproduction: identifies good solutions in a population makes multiple copies of the good solution eliminates bad solution

Cannot create new solution

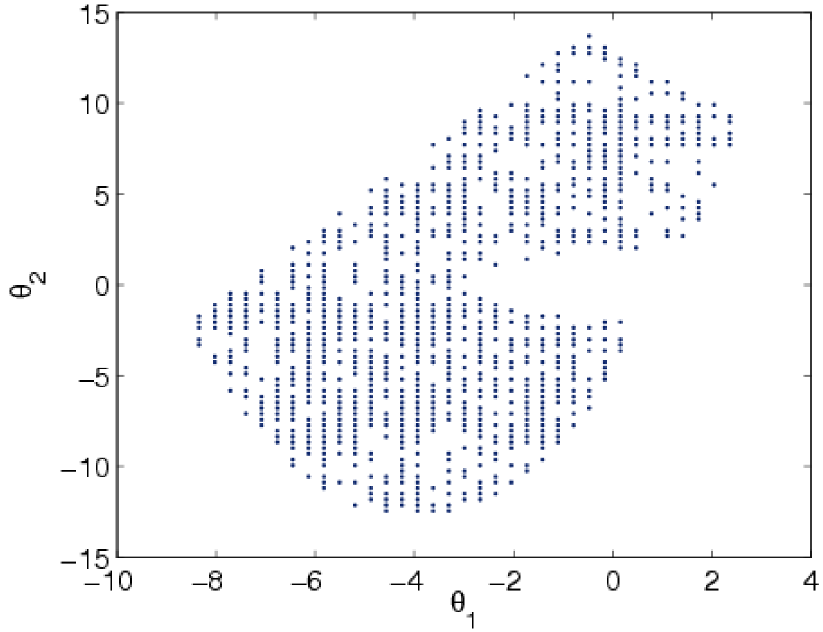
Crossover creates new solution by swapping portions of chromosomes

Number of strings with similarities at certain string position is increased

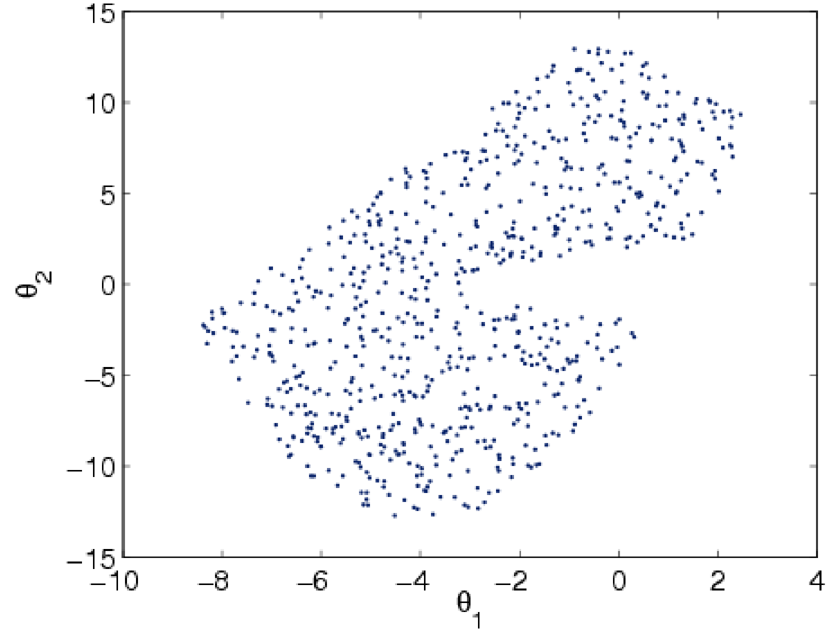
Schema

Performance of the Sampling Technique

Sampling using GA



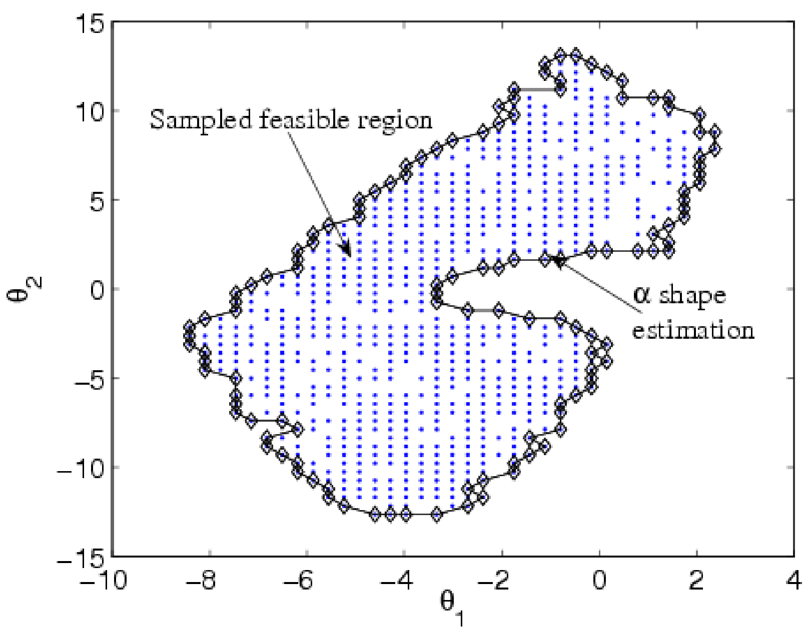
Simple Random Sampling



Population size = 20
Solution evolved for 2000 generations } 3000 function evaluations → ~ 1000 feasible points

Random Sampling : 950 feasible point generation required 10000 function evaluation

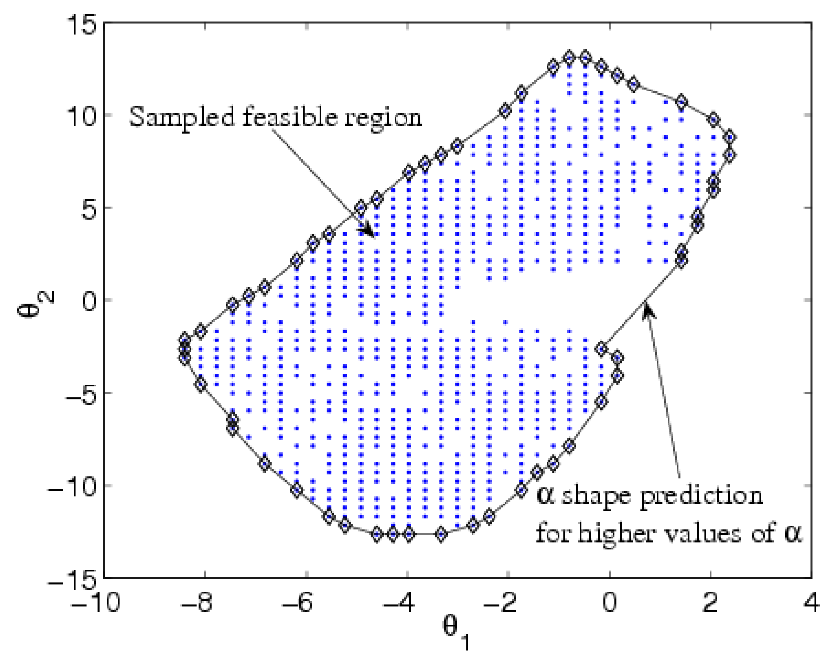
α – shape of the Sampled Data



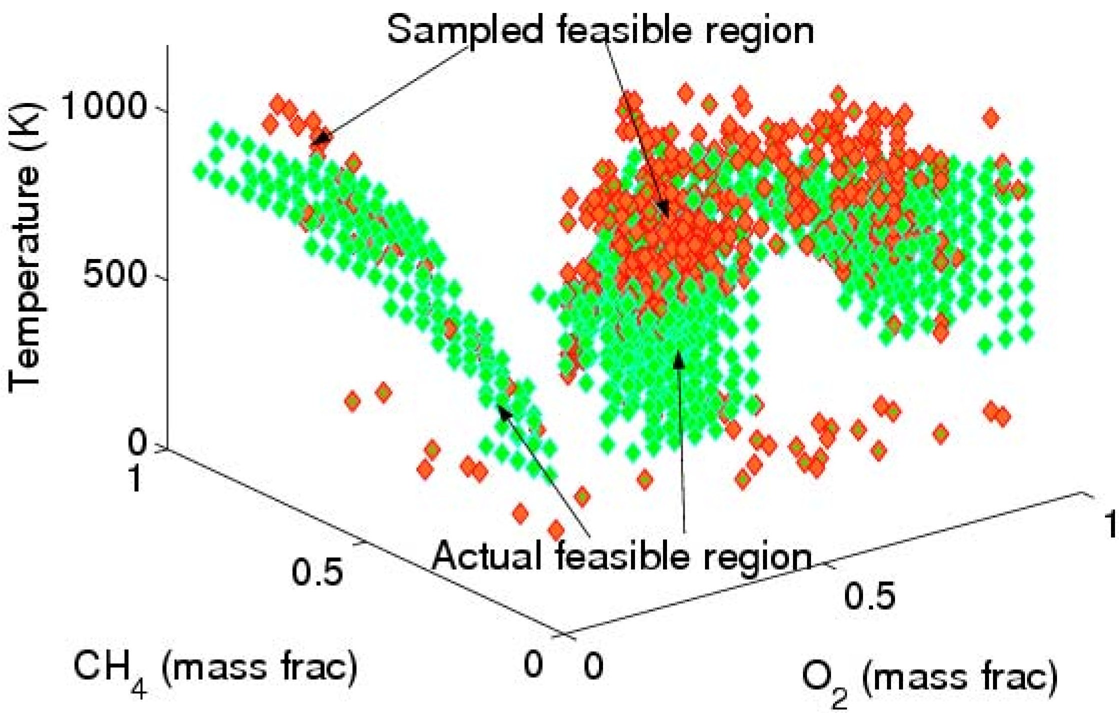
α value = $\sqrt{\frac{\mathcal{L}_n}{n}}$ ~ 25

α value of 25 accurately captured the non-convex shape

Higher value of α =1000 could not capture non-convexity



Estimation of Feasible Region: α -shape



Sample the feasible space by GA formulation

800 feasible points

GA : 1800 function evaluations

RS : 4000 function evaluations

Construct α – shape with the sampled points

Determine points forming the boundary of the feasible region

Join boundary points with triangle for polygonal representation of feasible region

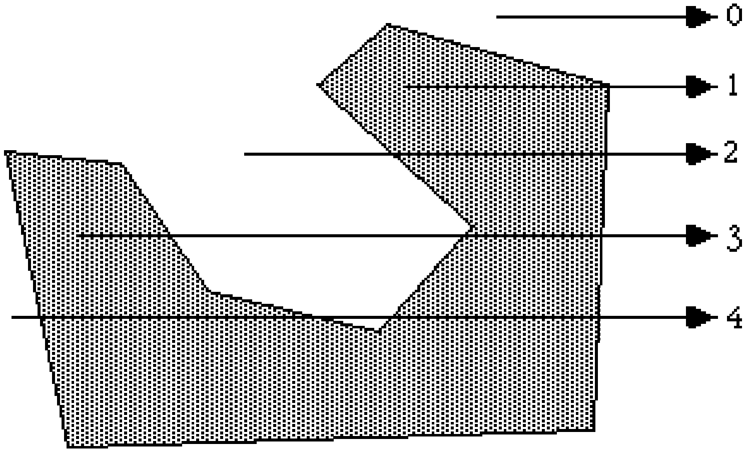
Determination of Feasible Conditions

Determination of conditions inside the feasible surface

Point-in-polygon algorithm

Ray casting algorithm

Jordan Curve Theorem



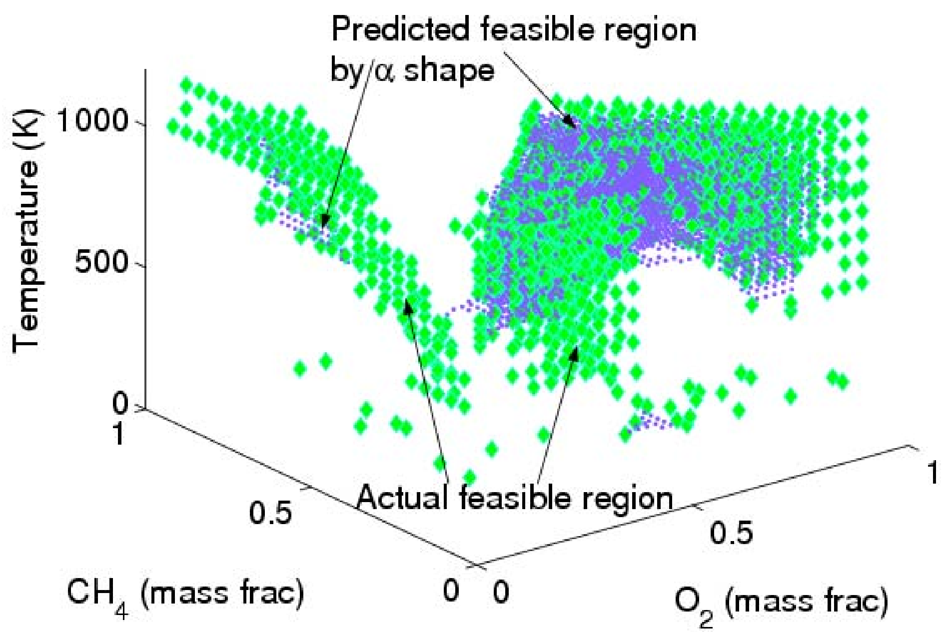
- Draw semi-infinite ray from point of concern
- Determine number of times it intersects surface

Point inside the surface → number of intersections odd

Point outside surface → number of intersections even/0

Perform point-in-polygon test to check if particular parameter value lies inside feasible region

Performance of α - shape



α – shape covers a larger region than convex hull

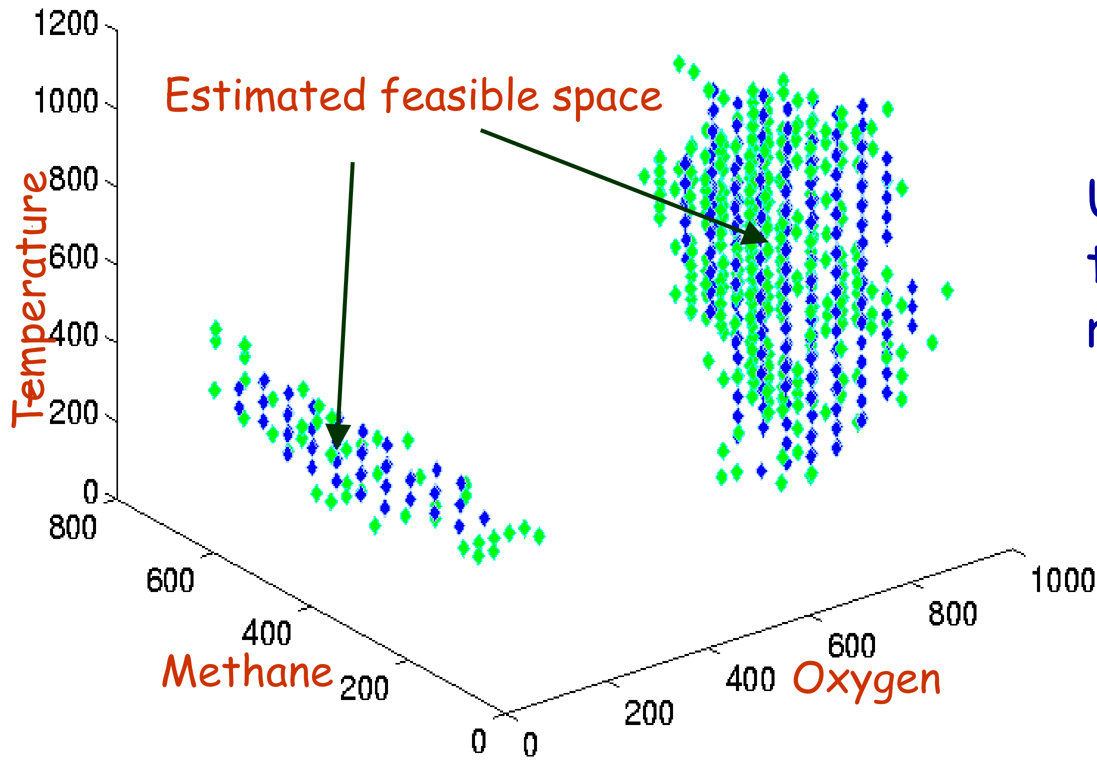
α - shape accurately captures the nonconvex shape

The prediction of feasible region by α - shape can be improved by a better sampling technique

Point-in-polygon check ~ 0.3 ms

α shape could capture ~ 80 % of the feasible region

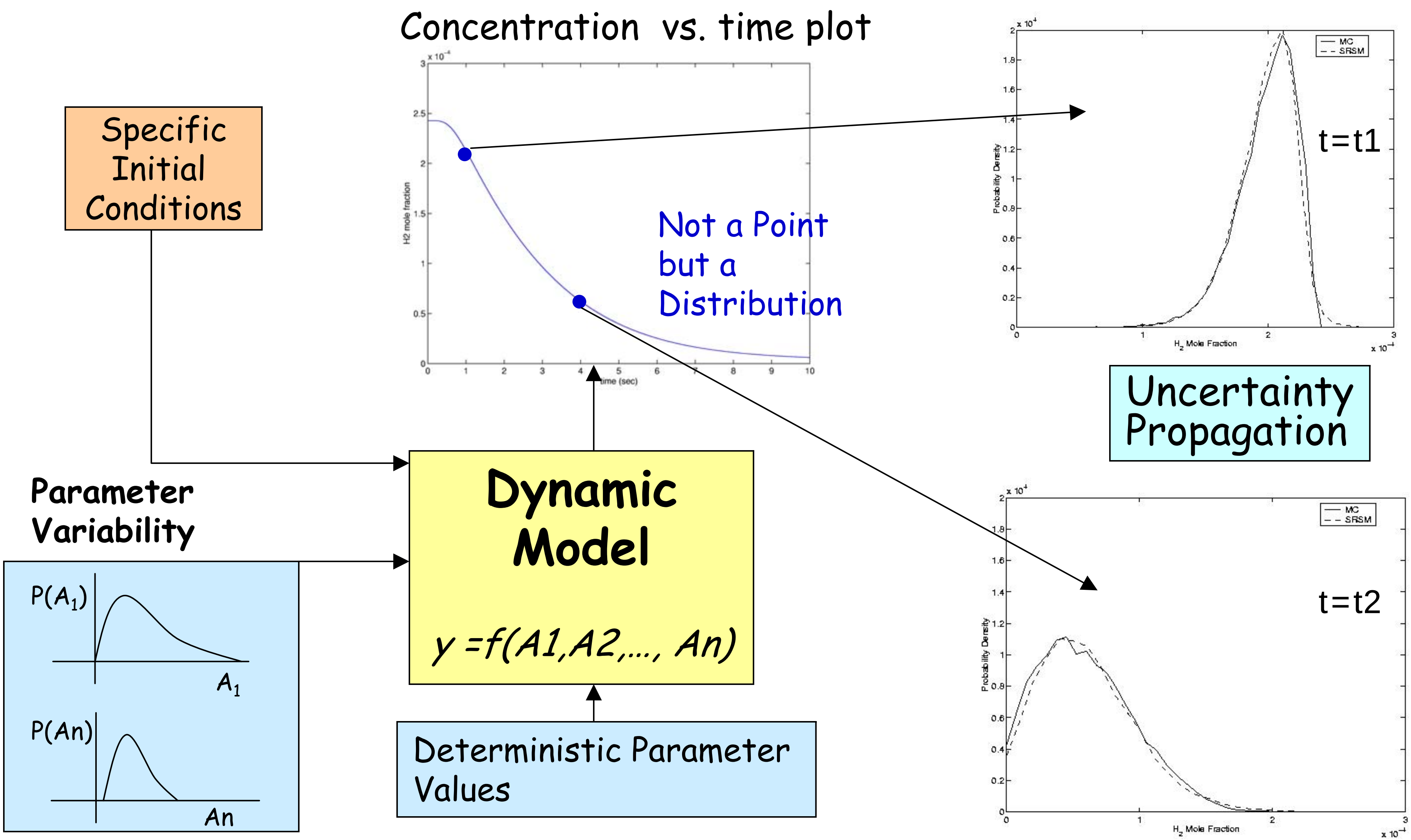
Capturing Disjoint Feasible Region by α - shape



Using α - shape it is possible to capture disjoint feasible regions

Characterizing the Effects of Uncertainty

Uncertainty Propagation



Stochastic Response Surface Method

- The outputs are represented as a polynomial chaos expansion (Ghanem and Spanos, 1991) in terms of Hermite polynomials :

$$U_1 = a_{0,1} + \sum_{i=1}^{n} a_{i,1}\xi_i \qquad \text{1}^{\text{st}} \text{ order}$$

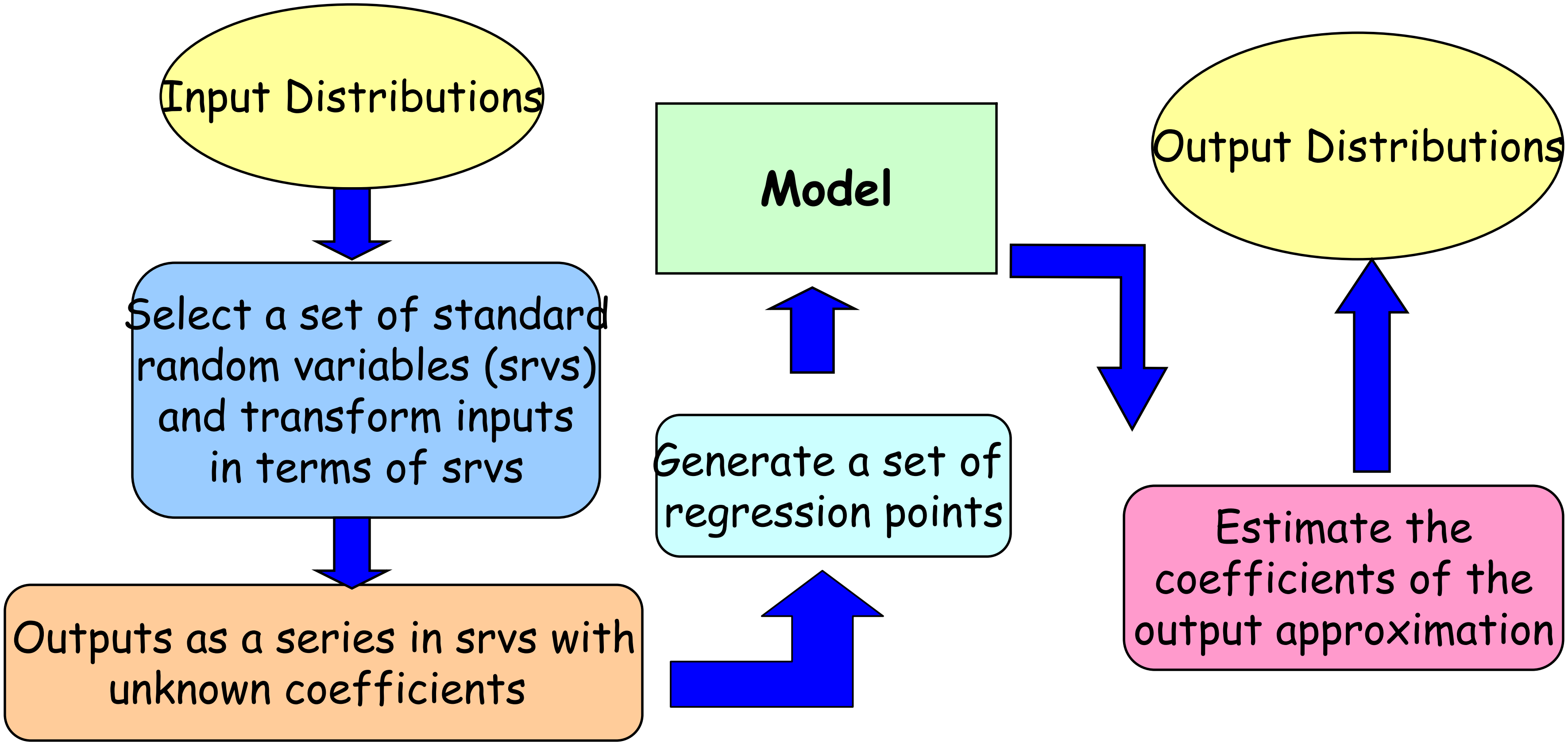
$$U_2 = a_{0,2} + \sum_{i=1}^{n} a_{i,2}\xi_i + \sum_{i=1}^{n} a_{ii,2}(\xi_i^2 - 1) + \sum_{i=1}^{n-1}\sum_{j>i}^{n} a_{ij,2}\xi_i\xi_j \qquad \text{2}^{\text{nd}} \text{ order}$$

- The coefficients of these polynomials are determined through application of an efficient collocation scheme and regression

- Direct evaluation of the output pdf's characteristics (for example, for a single variable second order SRSM approximation)

Mean = $a_{0,2}$ Variance = $a_{1,2}^2 + 2a_{11,2}^2$

Stochastic Surface Response Method



- **Two orders reduction in model runs required compared to Monte Carlo**
- **Output uncertainty expressed as polynomial function of input uncertainty**
- **Direct evaluation of the output pdf's characteristics**

Case Study : Supercritical wet oxidation

- Constant temperature (823K) high pressure (246 Bar) oxidation of H_2 and O_2 consisting of 19 reactions and 10 species
- Pre-exponential factors (A_i's) taken to be log-normal random variables. Parameters obtained assuming:
  - Computed and literature values of the multiplicative uncertainty factors (UF) valid for the reaction temperature considered
  - 95% confidence limits provide upper and lower bounds.

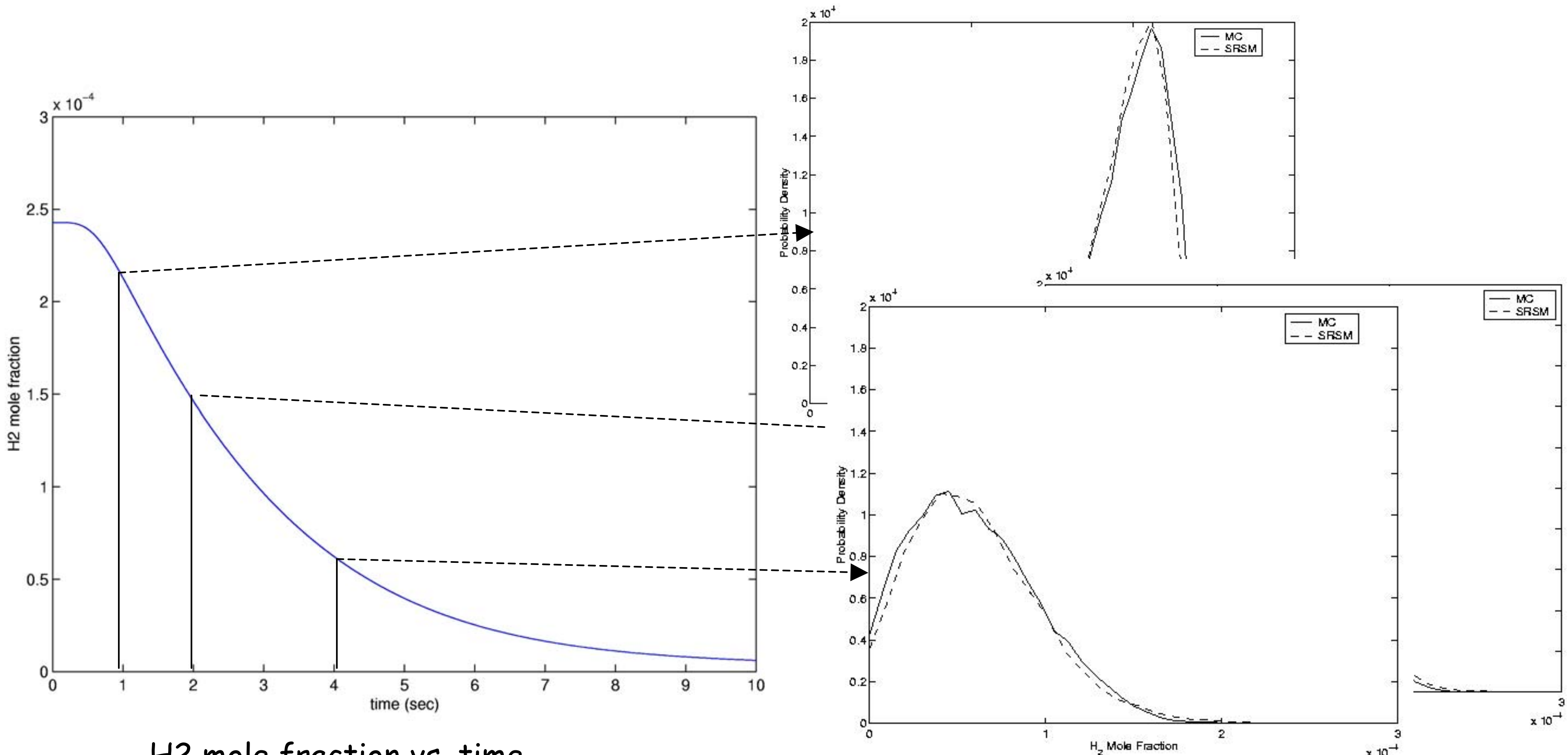
Reaction	$A_i$nom	n	E_a/R	UF_i
OH+H↔H2O	1.620E+14	0.00	75	3.16
H2+OH↔H2O+H	1.023E+08	1.60	1660	1.26
H+O2↔HO2	1.481E+12	0.60	0	1.58
HO2+HO2↔H2O2+O2	1.866E+12	0.00	775	1.41
H2O2+OH↔H2O+HO2	7.826E+12	0.00	670	1.58
H2O2+H↔HO2+H2	1.686E+12	0.00	1890	2.00
H2O2↔OH+OH	3.000E+14	0.00	24400	3.16
OH+HO2↔H2O+O2	2.890E+13	0.00	-250	3.16
H+O2↔OH+O	1.987E+14	0.00	8460	1.16
O+H2↔OH+H	5.117E+04	2.67	3160	1.22
2OH↔O+H2O	1.505E+09	1.14	50	1.22
H2+M↔H+H+M	4.575E+19	-1.40	52530	3.0
H+HO2↔OH+OH	1.686E+14	0.00	440	1.35
H+HO2↔H2+O2	4.274E+13	0.00	710	1.35
O+HO2↔OH+O2	3.191E+13	0.00	0	1.49
H2O2+H↔H2O+OH	1.023E+13	0.00	1800	1.35
O+H+M↔OH+M	4.711E+18	-1.00	0	10.0
O+O+M↔O2+M	1.885E+13	0.00	-900	1.3
H2O2+O↔OH+HO2	6.622E+11	0.00	2000	1.35

†Phenix et. al. 1998

Uncertainty Propagation: Results

(Balakrishnan S., P. Georgopoulos, I. Banerjee and M.G. Ierapetritou. *AIChE J*, **48** 2875, 2002)

- Concentration profiles display time varying distributions
- Number of model simulations required by SRSM is orders of magnitude less than Monte Carlo (723 vs. 15,000)

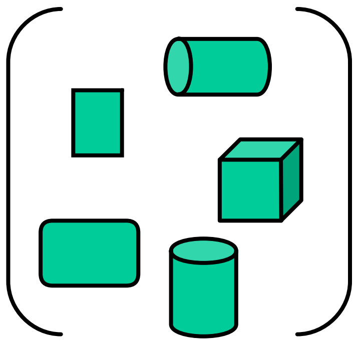


H2 mole fraction vs. time

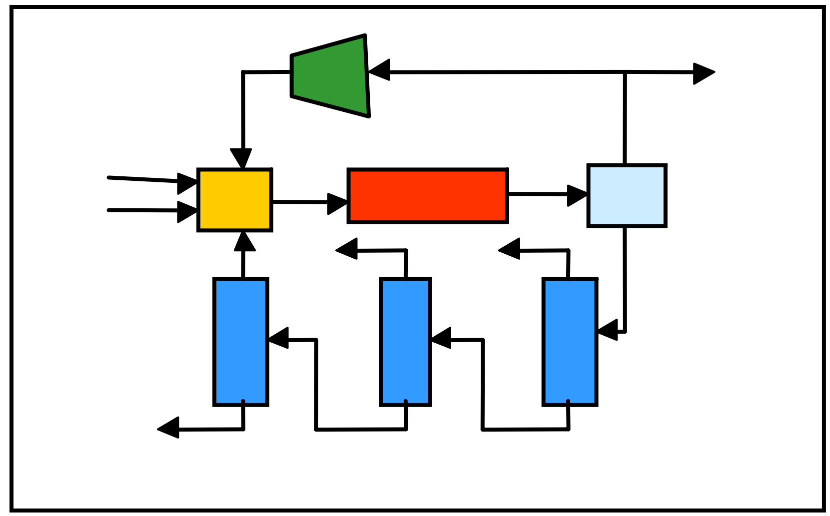
Design Considering Uncertainty

Process Design Considering Market Demand

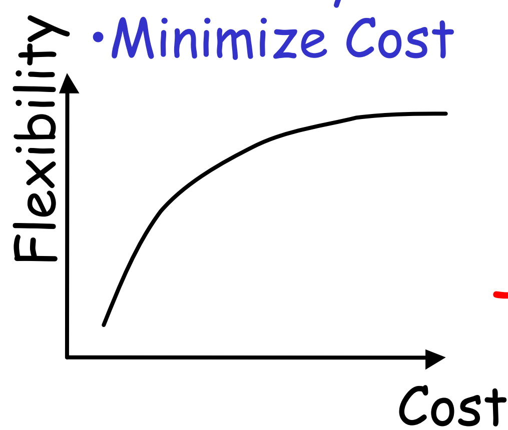
- Potential Set of Units
- Uncertainty in Internal And External Conditions



Flexible Production Plant



- Increase Plant Flexibility
- Minimize Cost



Trade-off : OPTIMIZATION

Objective: Develop a systematic methodology to increase the plant at a minimum cost

Background: Design Under Uncertainty

Existing approaches to model uncertainty in design/planning problem depends on nature of model equations *

Most models restricted by assumption of convexity *

Most models restricted to a rather small number of uncertain parameters

Require single model to describe uncertainty propagation irrespective of nature and complexity of the problem

*Gal,T.*Math.Prog.St.*(1984), Jongen,H.T.,Weber,G.W. *Ann. Op. Res.* (1990), Pistikopoulos and coworkers,

Background : Design under Uncertainty

Deterministic Approach : description of uncertainty is provided by specific bounds, or finite number of fixed parameter values

Grossmann, Halemane, AIChE (1982); Grossmann, Sargent AIChE (1987)

Stochastic Approach : uncertainty described by probability distribution functions

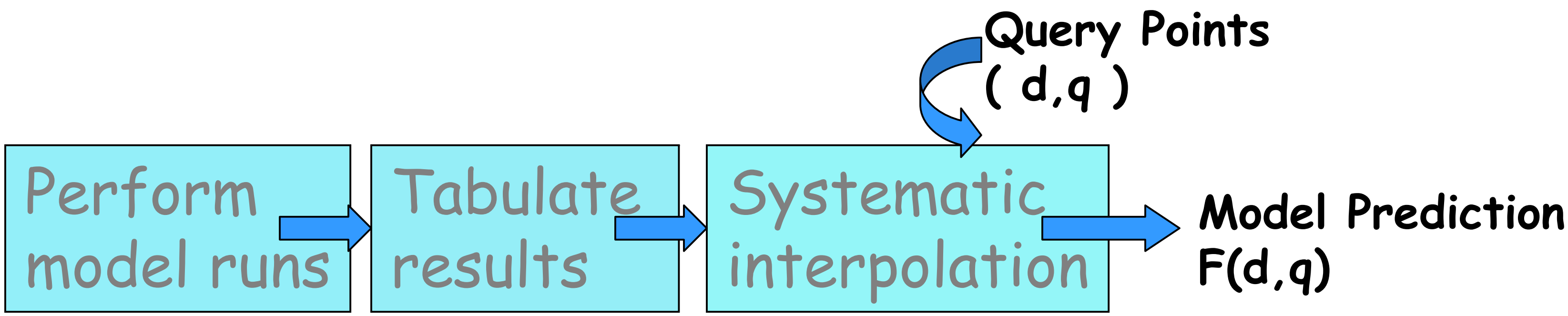
Pistikopoulos, Mazzuchi, Comput. Chem. Engg.(1990)

Combined multiperiod/ stochastic formulation : combines parametric and stochastic programming approaches to deal with synthesis/planning problems

Ierapetritou et al, Comput. Chem. Engg (1996), Hene et al, I&ECR (2002)

Proposed Technique

Tabulation technique to map input uncertainty to model output.



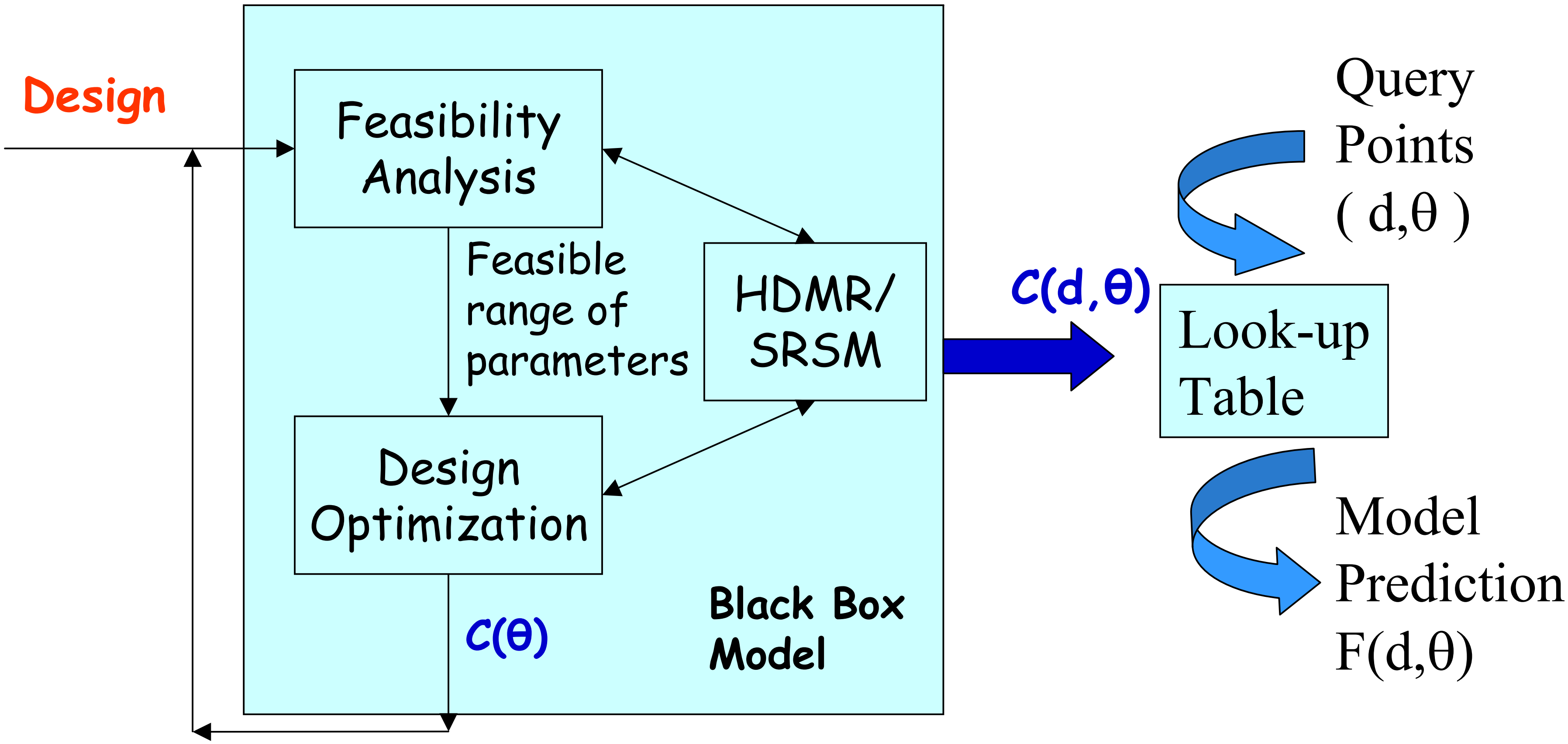
High Dimensional Model Representation (HDMR)* technique used to capture the variations of output with changes in the input

** Rabitz,H. Alis,O. J. Math. Chem. 25,195(1999)*

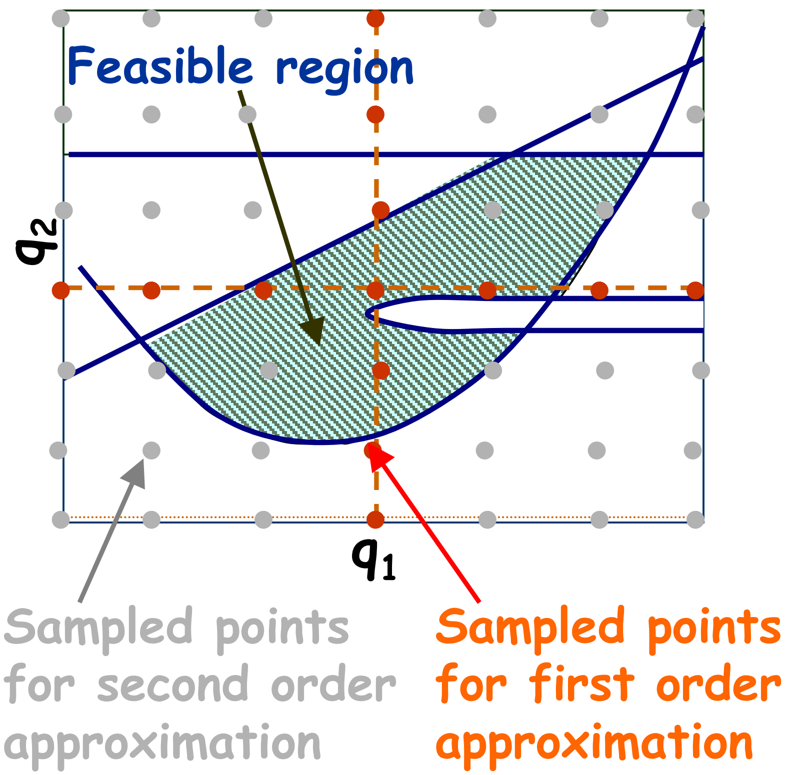
Design with Parametric Uncertainty:Blackbox Models

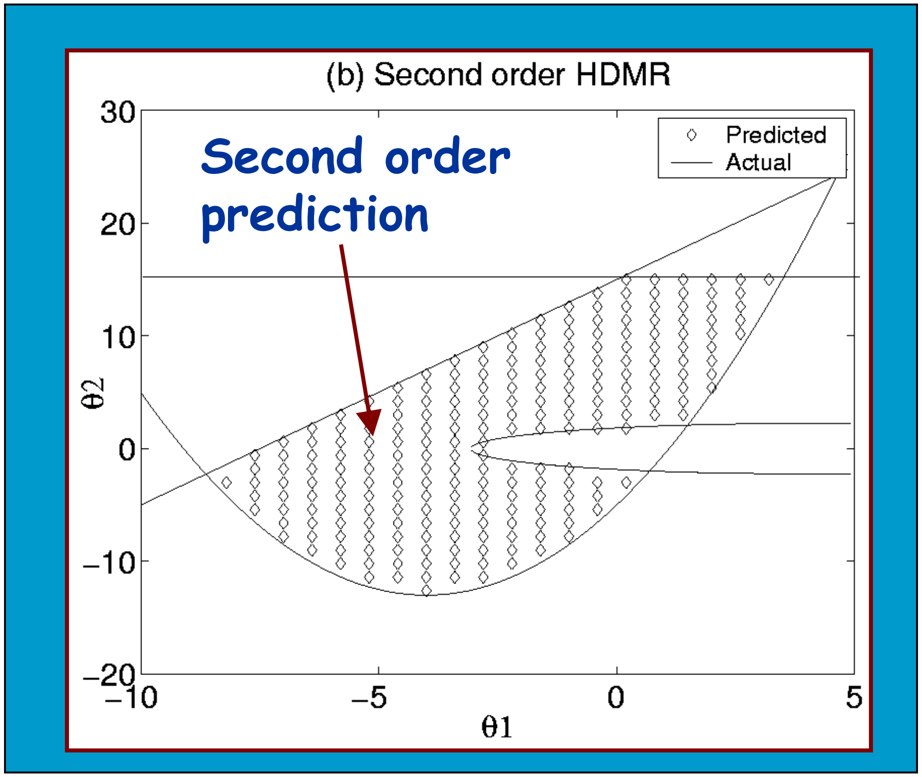
(Banerjee, I., and M.G. Ierapetritou. *Ind. & Eng. Chem. Res*, **41**, 6687, 2002)

- **No Assumptions** Regarding System's Model
- **Parametric Expression** of the Optimal Solution



Feasibility Analysis





High Dimensional Model Reduction

$$g(x_1, x_2, \ldots x_n) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1 \le i < j \le n}^{n} f_{ij}(x_i, x_j) + \ldots + f_{1,2,\ldots n}(x_1, x_2, \ldots, x_n)$$

f_0 constant

$f_i(x_i)$ independent action of variable x_i upon the output

$f_{ij}(x_i, x_j)$ correlated impact of x_i, x_j upon the output

. . .

$f_{1,2,\ldots,n}(x_1, x_2, \ldots, x_n)$ residual correlated impact

- Order of correlation of independent variables diminish rapidly
- 2nd order approximation commonly suffices
- Application in complex kinetics modeling (i.e.,atmospheric chemistry, photochemical reaction modeling etc)

Evaluation of first order expansion function requires $n(s-1)$ model runs
Evaluation of second order expansion requires $n(s-1)^2(n-1)/2$ model runs

Nonlinear Multiparametric Problem

Optimization problem

Min z

Subject to :

$$-z-\theta_1+\theta_2^2/2+2\theta_3^3+d_1-3d_2-8 \le 0$$

$$-z-\theta_1/3-\theta_2-\theta_3/3+d_2+8/3 \le 0$$

$$z+\theta_1^2-\theta_2-d_1+\theta_3-4 \le 0$$

Feasibility problem

Min u

Subject to :

$$-z-\theta_1+\theta_2^2/2+2\theta_3^3+d_1-3d_2-8 \le u$$

$$-z-\theta_1/3-\theta_2-\theta_3/3+d_2+8/3 \le u$$

$$z+\theta_1^2-\theta_2-d_1+\theta_3-4 \le u$$

Where:
z is control variable.
q_1, q_2, q_3 are uncertain parameters.
d_1,d_2 are design variables.

$\theta_1 \in [0\ 4]$; $\theta_2 \in [0\ 4]$; $\theta_3 \in [0\ 4]$
$d_1 \in [1\ 5]$; $d_2 \in [1\ 5]$

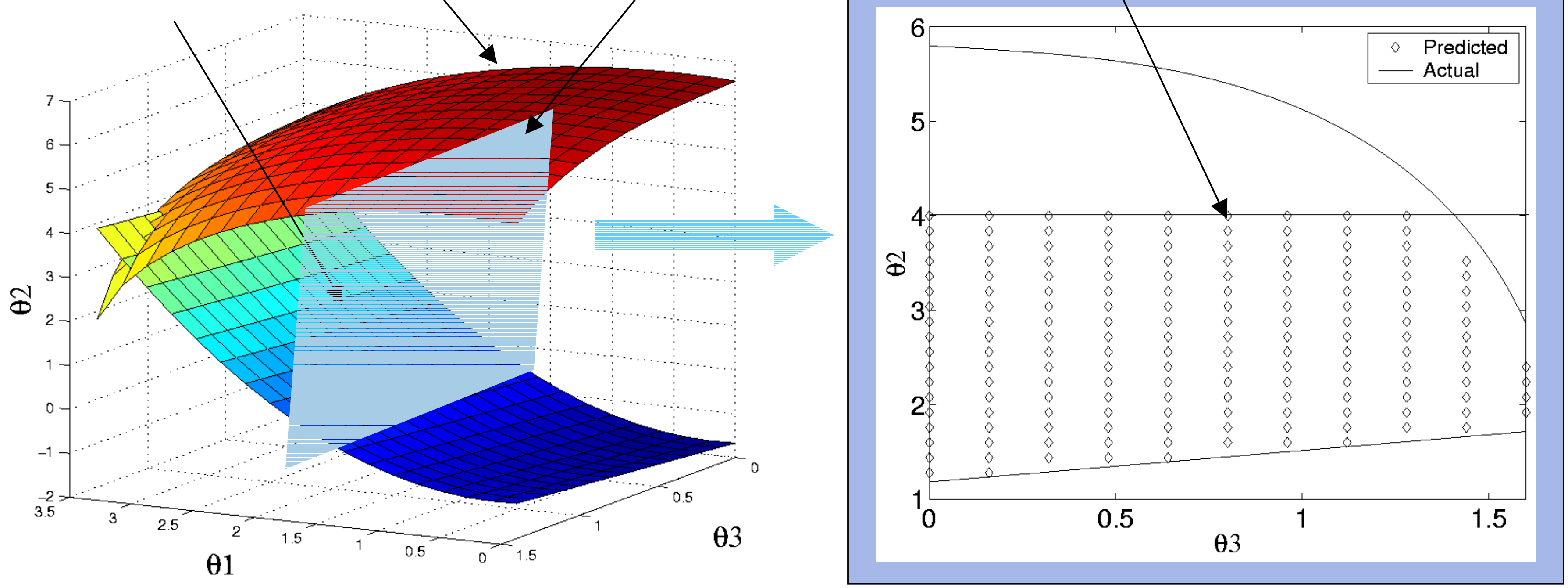
Steps of Proposed algorithm:Feasibility Analysis

Step 1:
Fix the value of design variable. Determine the feasible region of operation.

Constraints bounding the feasible region

Fixed value of θ_1=2.56

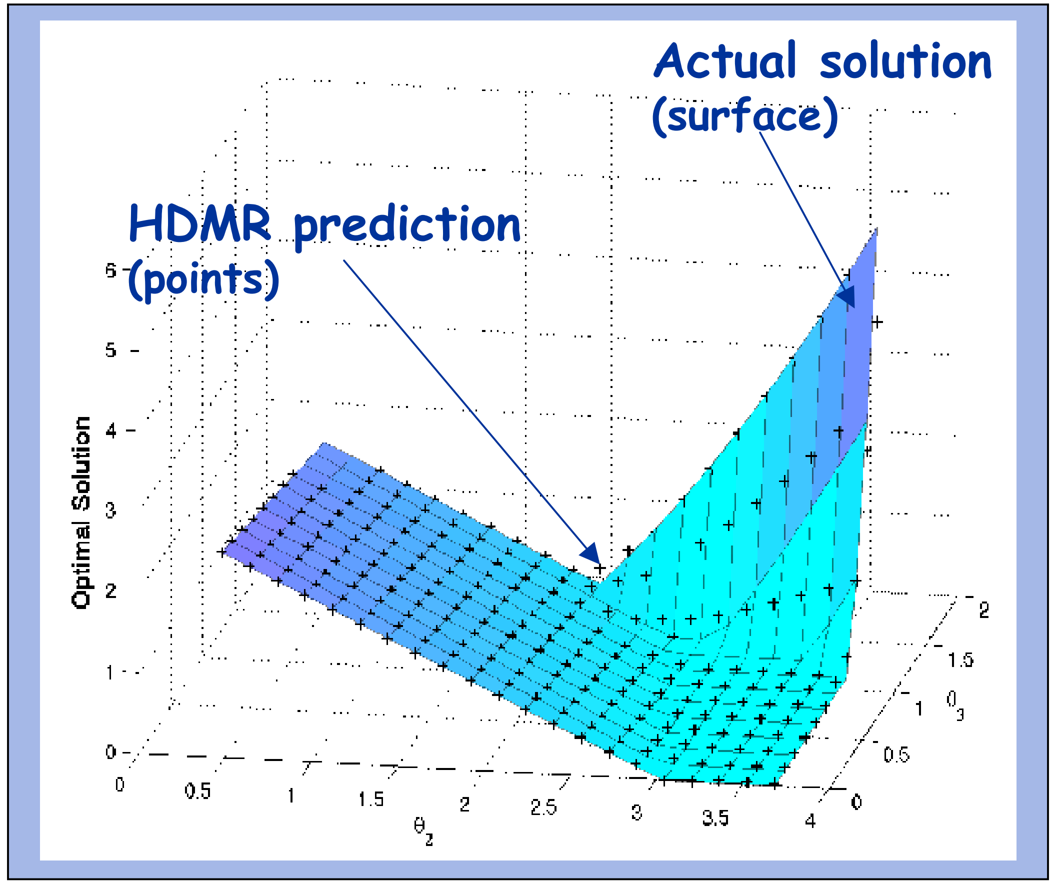
HDMR prediction



No overprediction; 0.7% underprediction

Steps of Proposed Algorithm: Optimization Problem

Step 2 :
Determine the variation of optimal solution with uncertain parameters for the fixed value of design



Estimation Error = 3.73 %

Steps of Proposed Algorithm: Design Problem

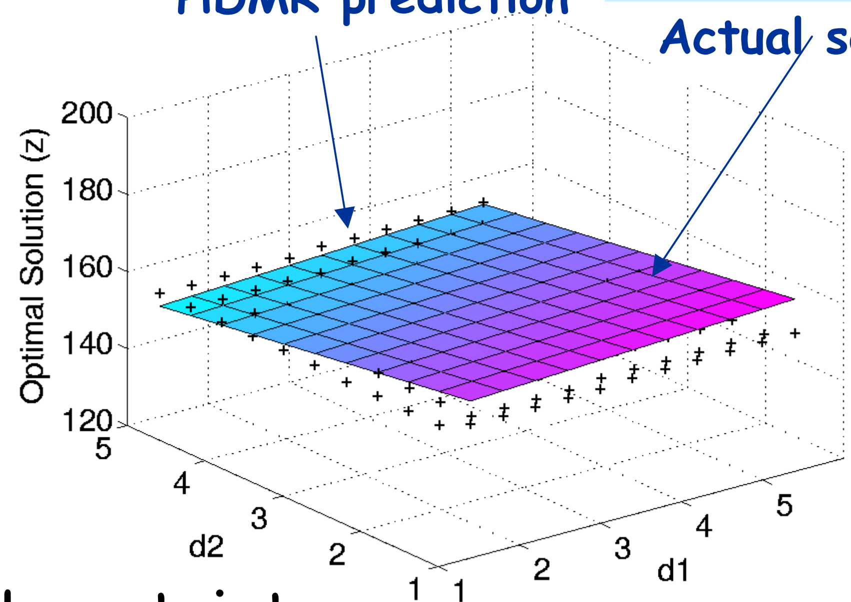
Step 3 :
Perform the feasibility analysis and design optimization for different values of design variables.

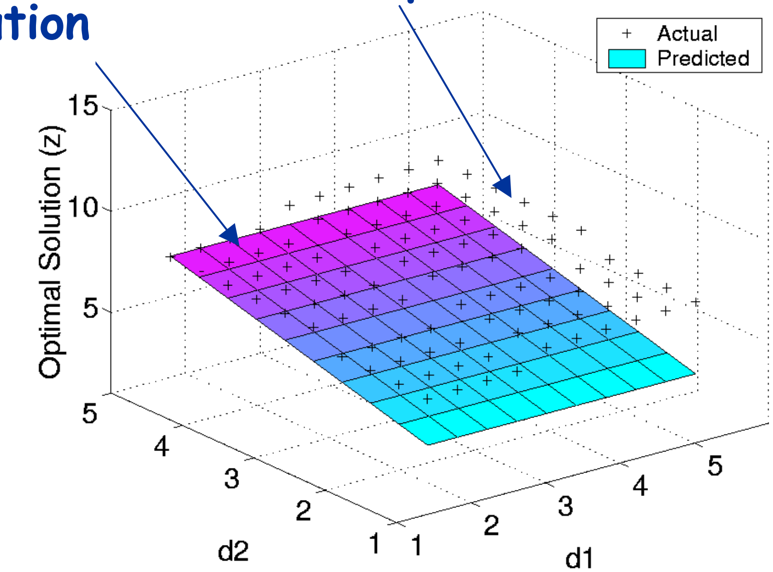
Estimation Error 7%

HDMR prediction

Actual solution

HDMR prediction

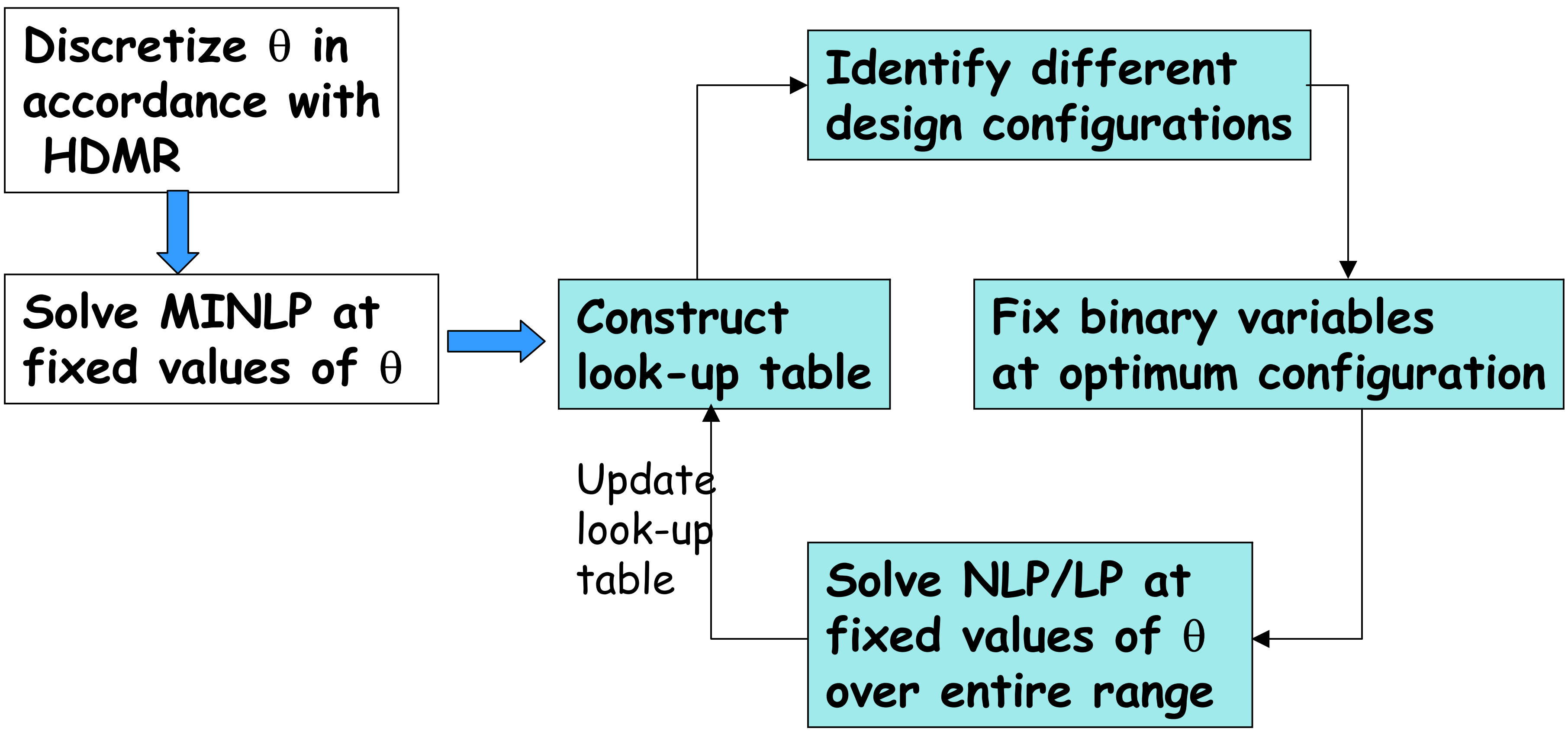




Uncertainty at the mean Error=0.4%

Uncertainty at the extreme Error=5.5%

Process Synthesis Problem



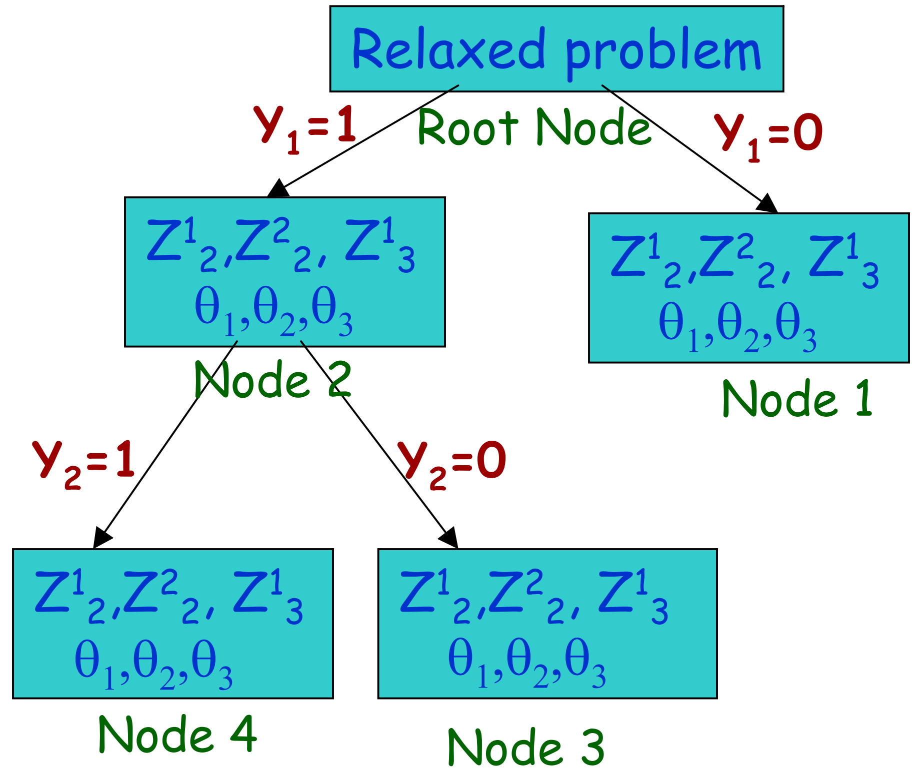
Branch and Bound Procedure

Binary variables : y1,y2

Uncertain parameters : θ

At each node solve NLP/LP
at fixed values of θ $(\theta_1,\theta_2,\theta_3)$

Branching criteria:
Choose a node having larger
number of better optimal solutions



Fathoming criteria:
Compare solutions at all θ values.
Fathom a node with respect to a particular θ value.

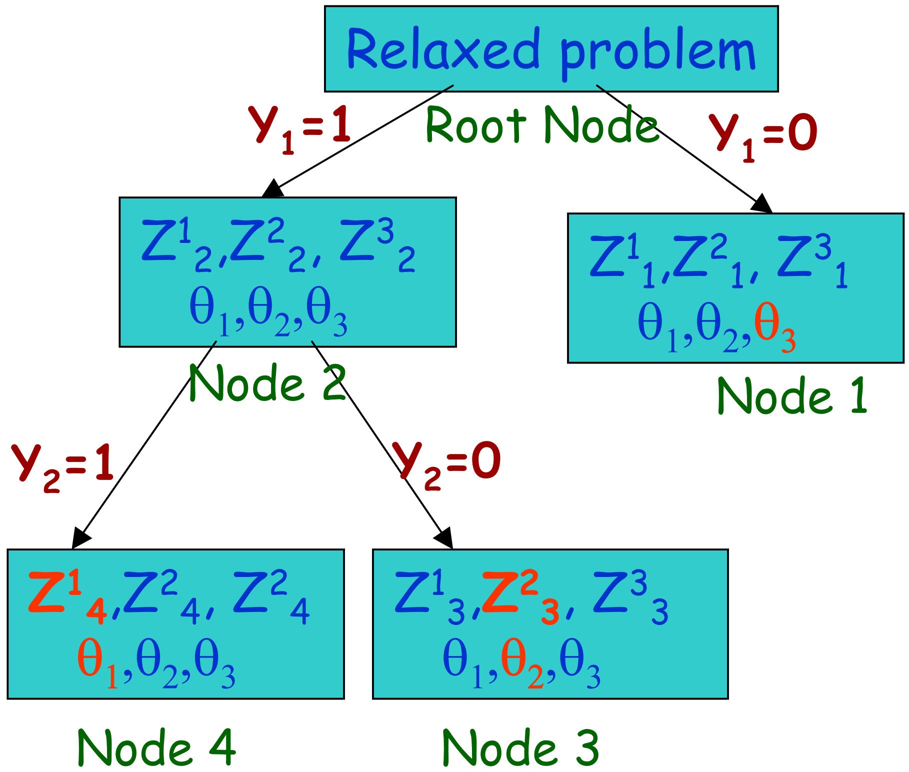
Branch and Bound Procedure (Example)

Branching Step :
Compare solutions of Node 1 and Node 2
$z^1_2 > z^1_1$; $z^2_2 > z^2_1$; $z^3_2 < z^3_1$
Selected node for branching: Node 2

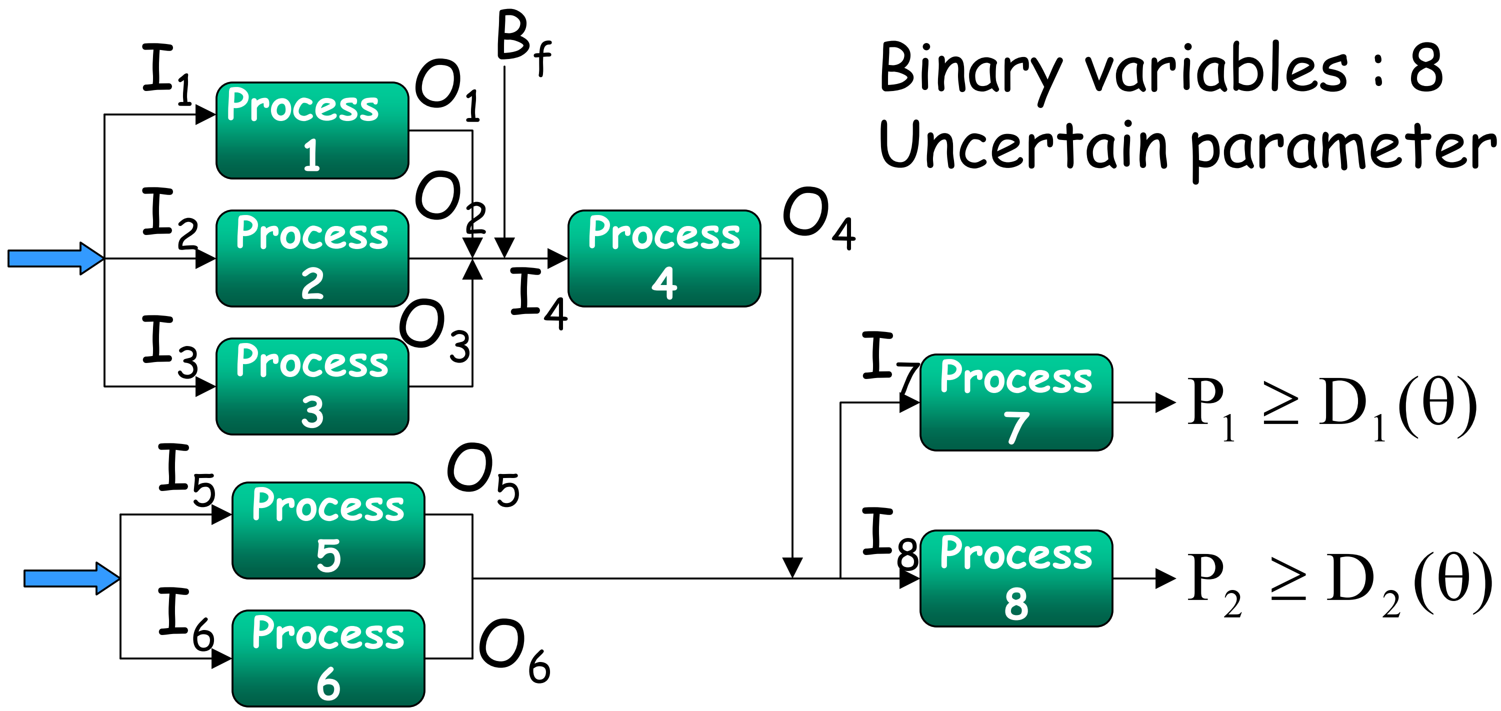
Fathoming Step:
Compare Node 3 and Node 4
$z^1_4 > z^1_3$; $z^2_4 < z^2_3$; $z^3_4 < z^3_3$
Compare Node 3 and Node 1
$z^1_3 > z^1_1$; $z^2_3 > z^2_1$; $z^3_3 < z^3_1$

Optimal solution
At θ_1 : z^1_4 [1,1] ; At θ_2 : z^2_3 [1,0]

Fathom Node 1 wrt θ_1,θ_2
Branch on Node 1 only for θ_3



Example Problem with Single Uncertain Parameter

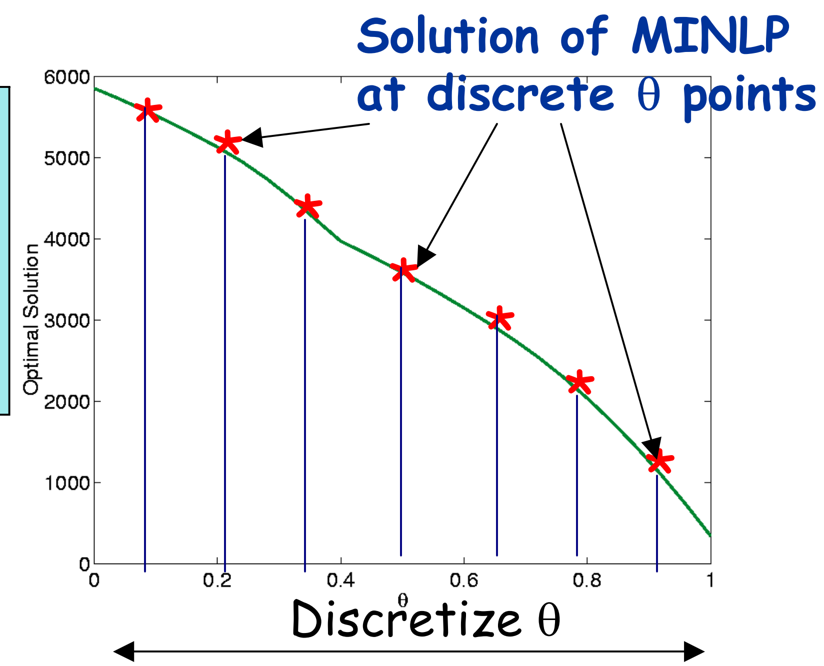


Binary variables : 8
Uncertain parameter : 1

* *Acevedo and Pistikopoulos 1996*

Application of the Proposed Approach

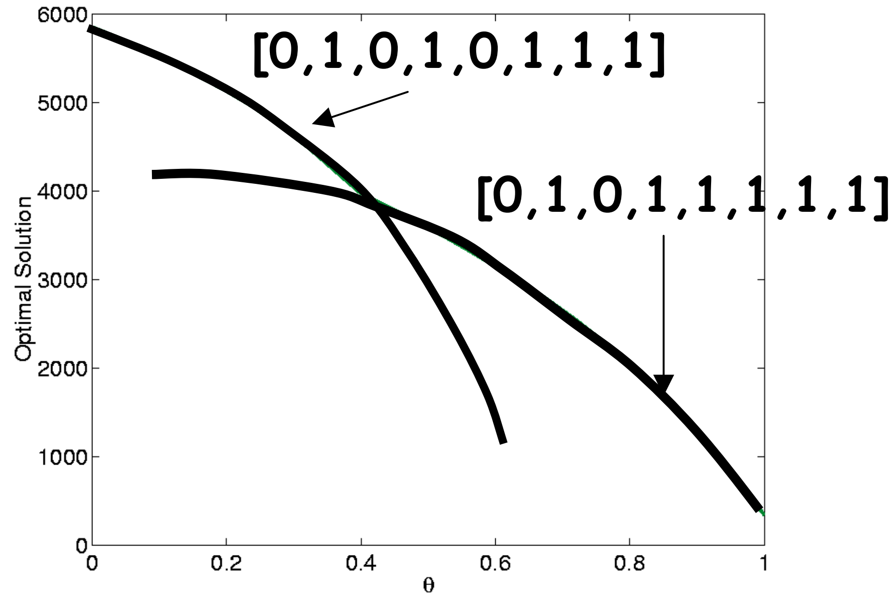
Step 1:
Uncertain range of θ discretized.
MINLP solved at each discrete θ value.



Optimal binary solutions are noted
[0,1,0,1,0,1,1,1] [0,1,0,1,1,1,1,1]

Application of the Proposed Approach

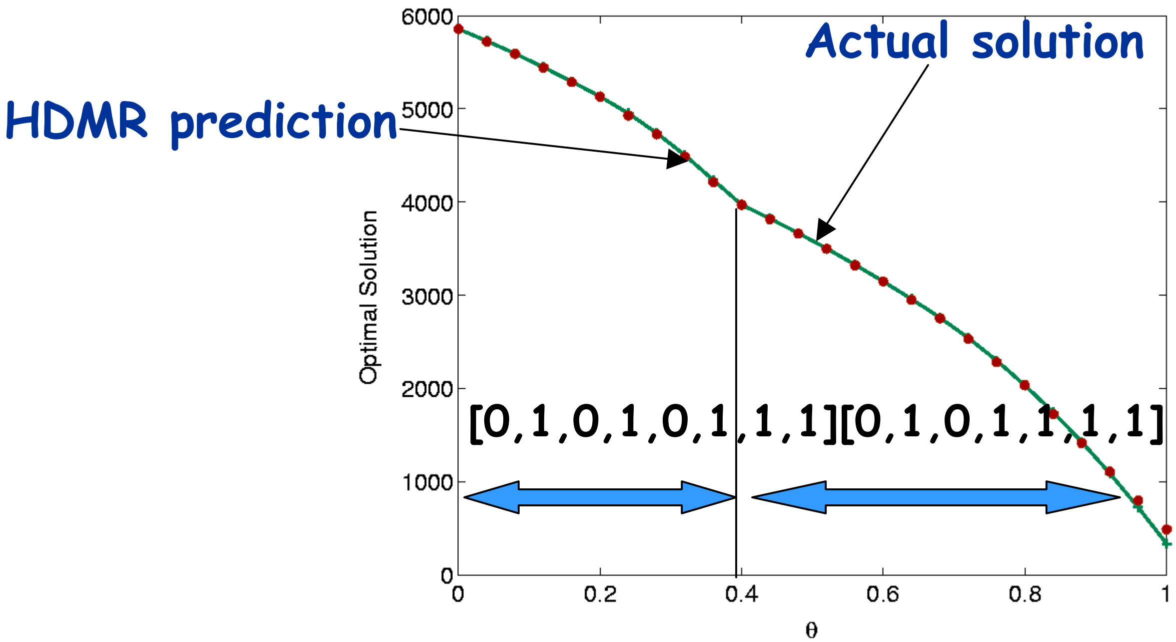
Step 2:
Fix binary variable at optimal combination.
Solve NLP/LP at different θ values over entire range of θ



Predict variation of optimal solution for each binary combination over entire range of θ

Application of the Proposed Approach

Analyze predicted variation of optimal solution to determine optimal binary configuration and optimal solution



Estimation Error = 1.7%

Error Analysis of Process Synthesis Problem

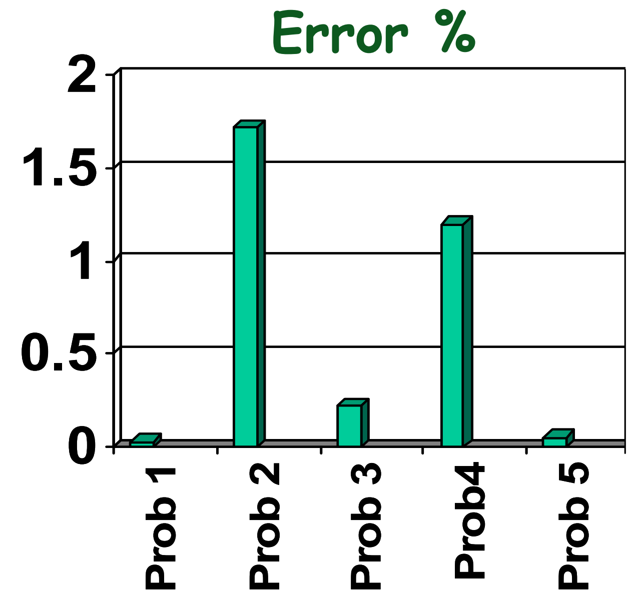
Problem 1(linear):
3 Binary variables ; 1 uncertain parameter

Problem 2 (nonlinear):
8 Binary variables; 1 Uncertain parameters

Problem 3 (nonlinear):
8 Binary variables; 2 Uncertain parameters

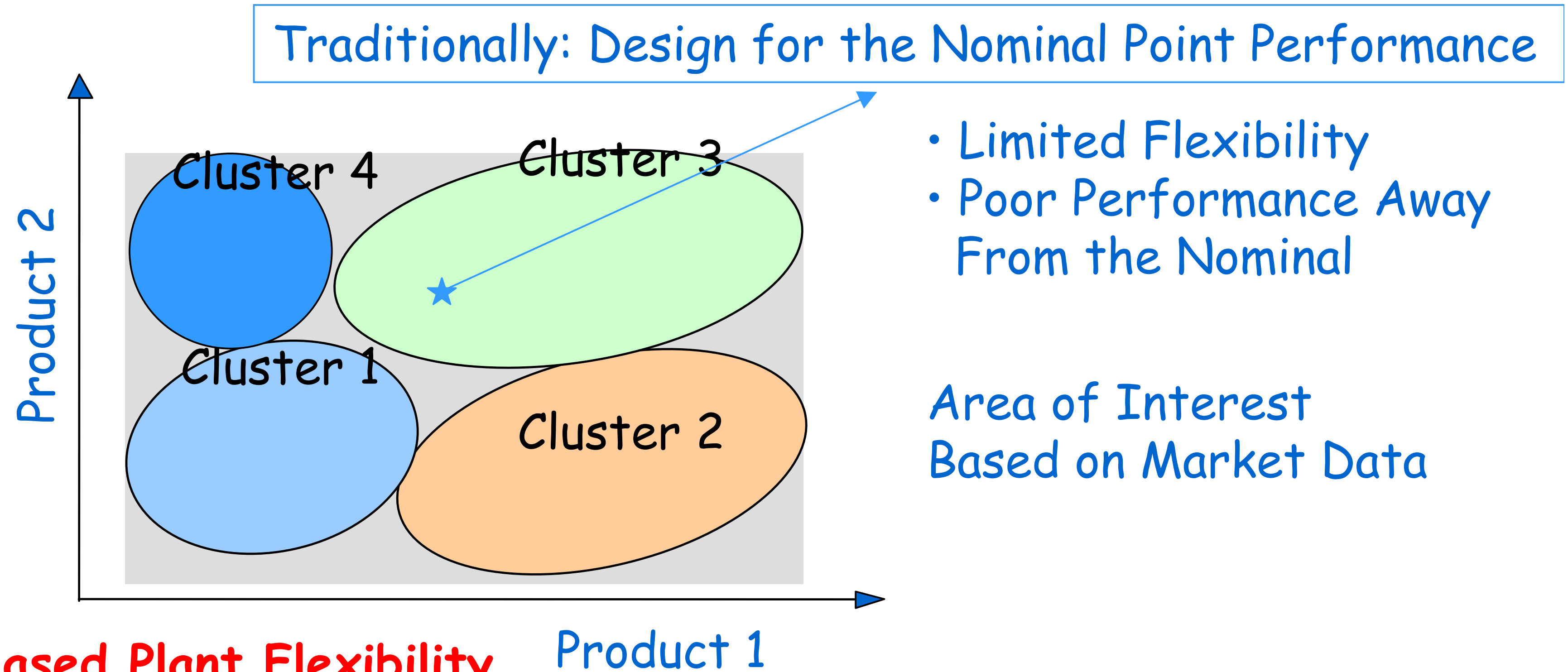
Problem 4(linear):
2 Binary variables; 3 Uncertain parameters

Problem 5 (nonlinear):
6 Binary variables; 3 Uncertain parameters



Design Optimization Integrating Market Data

Integration of Data Analysis,and Feasibility Quantification at the Process Design

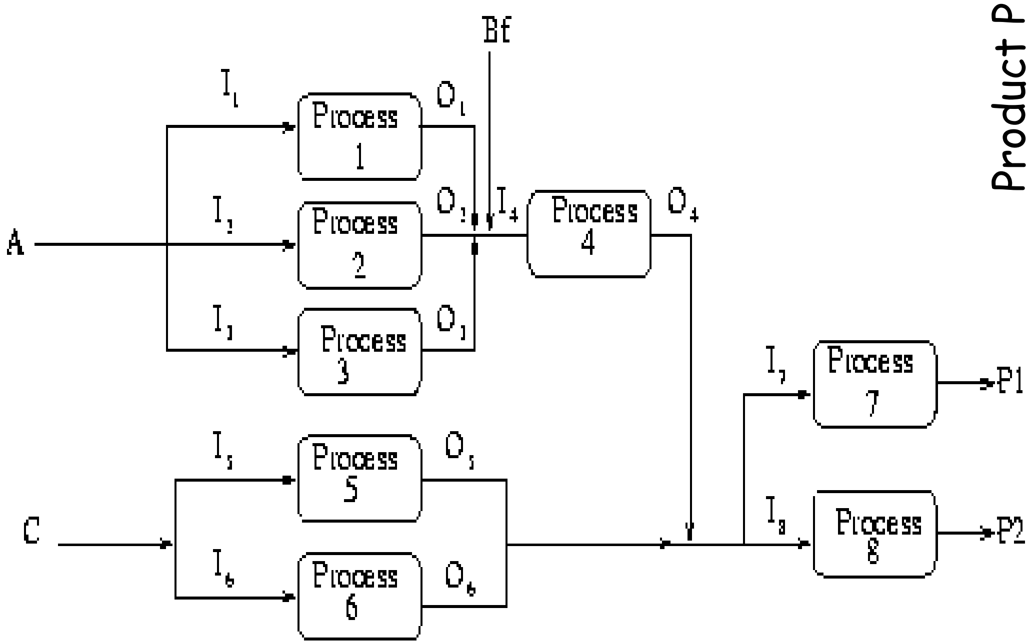


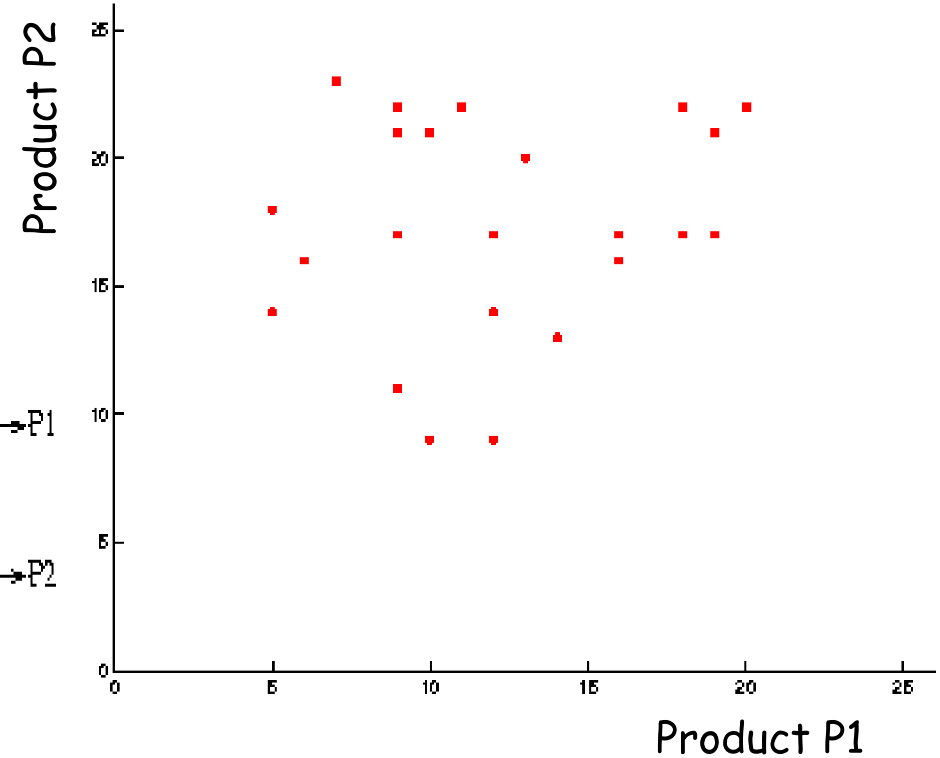
- Limited Flexibility
- Poor Performance Away From the Nominal

Area of Interest Based on Market Data

- **Increased Plant Flexibility**
- **Better Performance Within the Whole Range of Interest**
- **Larger Profitability Due to the Economy of Scale**

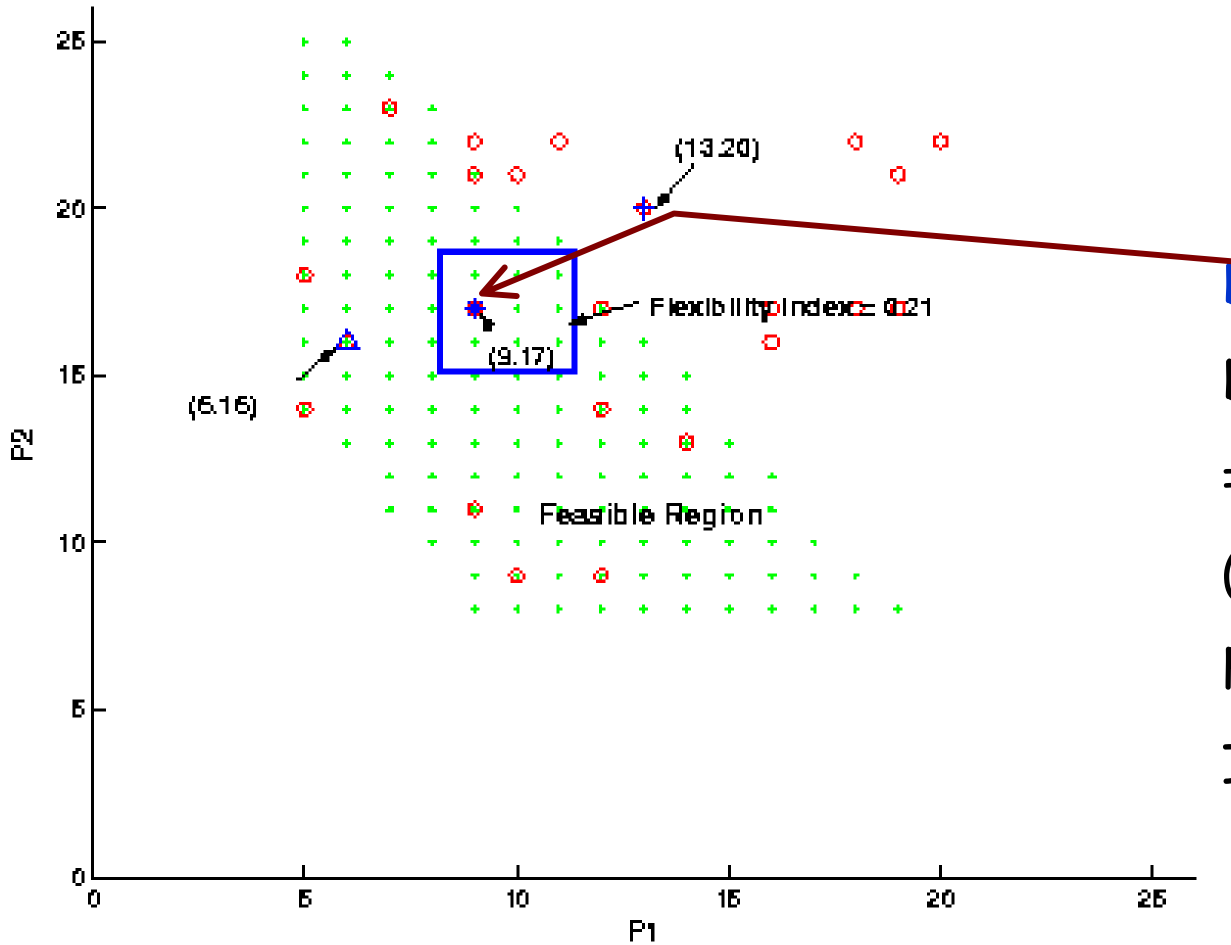
Motivation Example





- ❑Produce P_1 and P_2 from A,B,C
- ❑Given Demand Data for P_1 and P_2
- ❑ MINLP Optimization

Flexibility Plot for Customized Design Development



Demand = (9,17)

Design configuration

= (1,0,0,1,0,0,1,1)

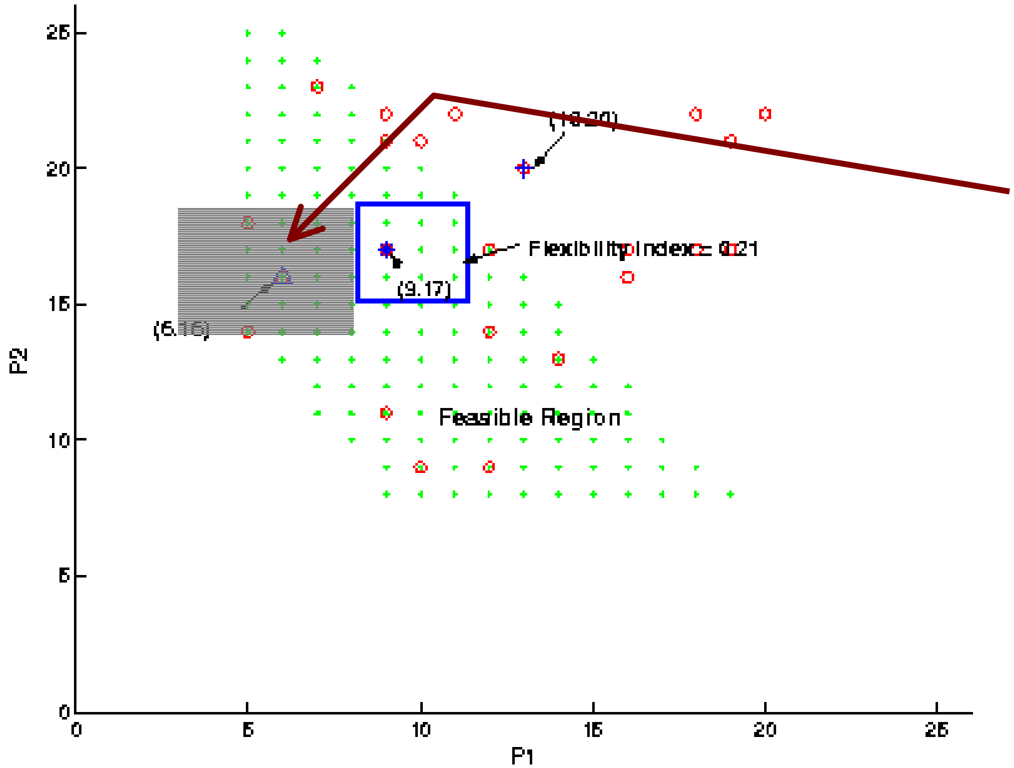
(Processes 1, 4, 7, 8)

Flexibility

Index = 0.21

Limitations -1

Underestimation of the Feasible Region



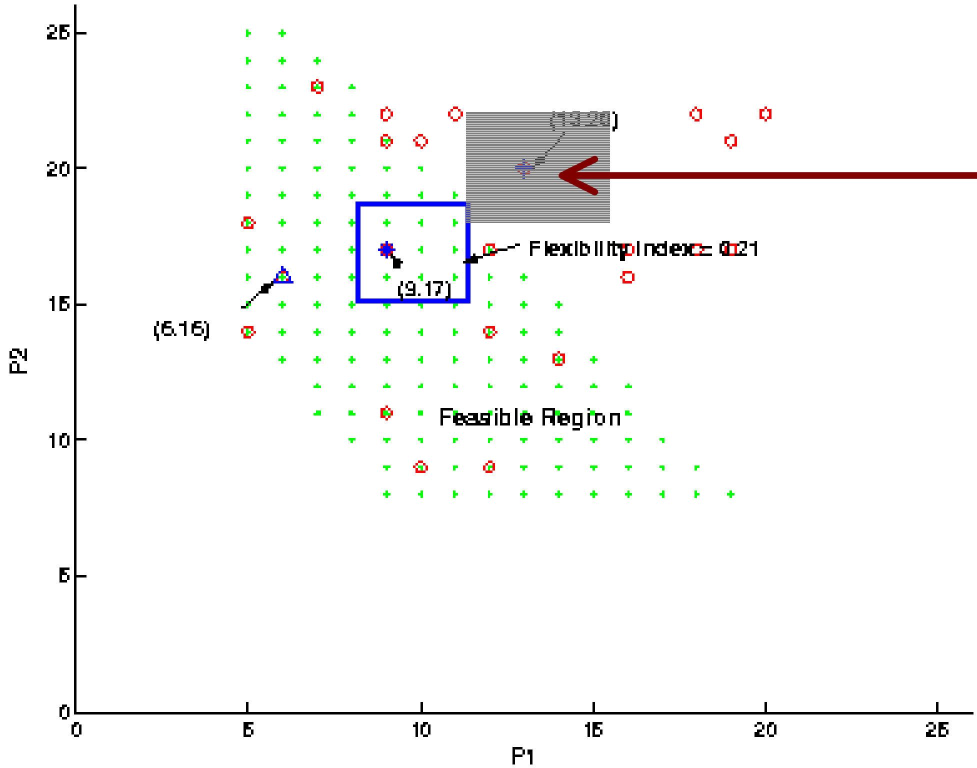
Demand point (6,16)

Feasible

No New Design Needed

Limitations -2

Customized Design Development



Demand point (13,20)

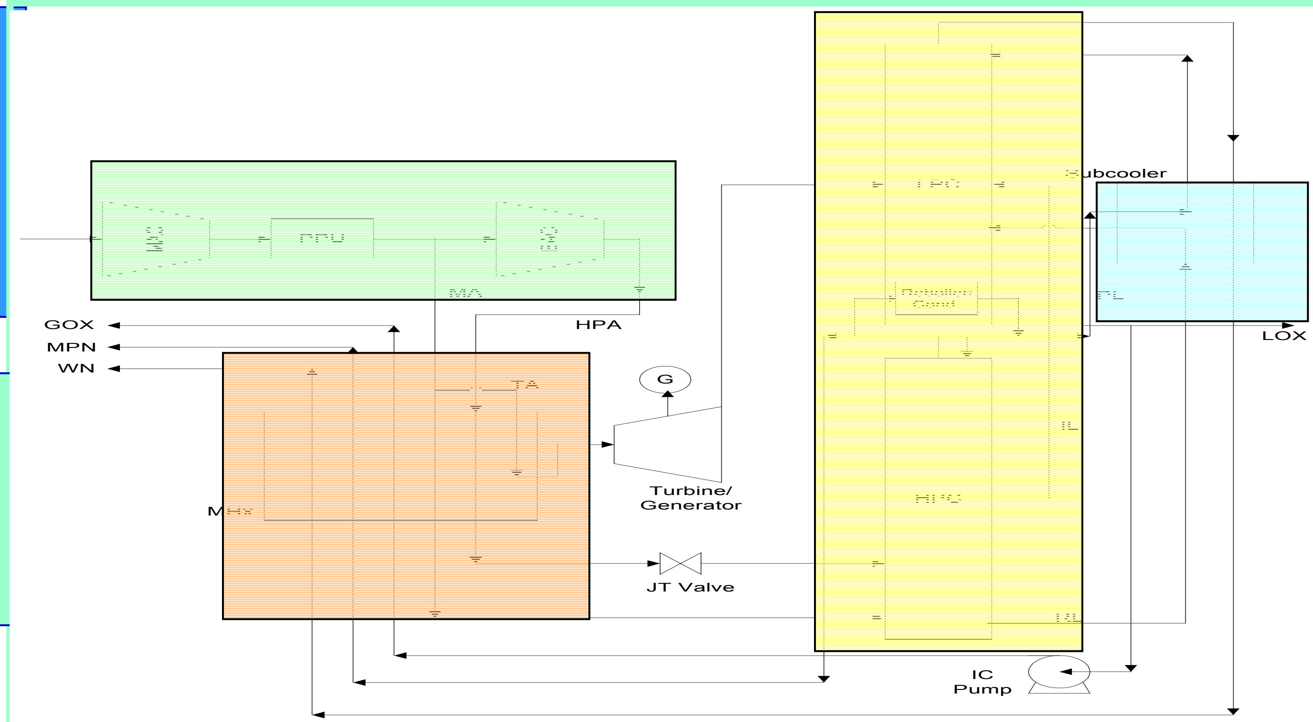
New Design Required

Moving the System Boundaries

Supply chain information

Given:
- Ranges of product quality
- Ranges of throughput
- Design alternatives

Given:
- Product specifications of different clients
- Client expectations



Find: the set of designs that optimally cover the whole space

Required Tools

- Accurate description of the feasible space of a process
- Data Clustering technique to cluster the demand data into closely packed groups
- Development of a unified data analysisprocess optimization framework

Data Analysis (Clustering)

- Partition a data set of multi-dimensional vectors into clusters such that patterns within each cluster are more "similar" to each other than to patterns in other clusters.

- Quality of Clustering depends on both the similarity measure used by the algorithm and its implementation.

K-Medoid Clustering: PAM

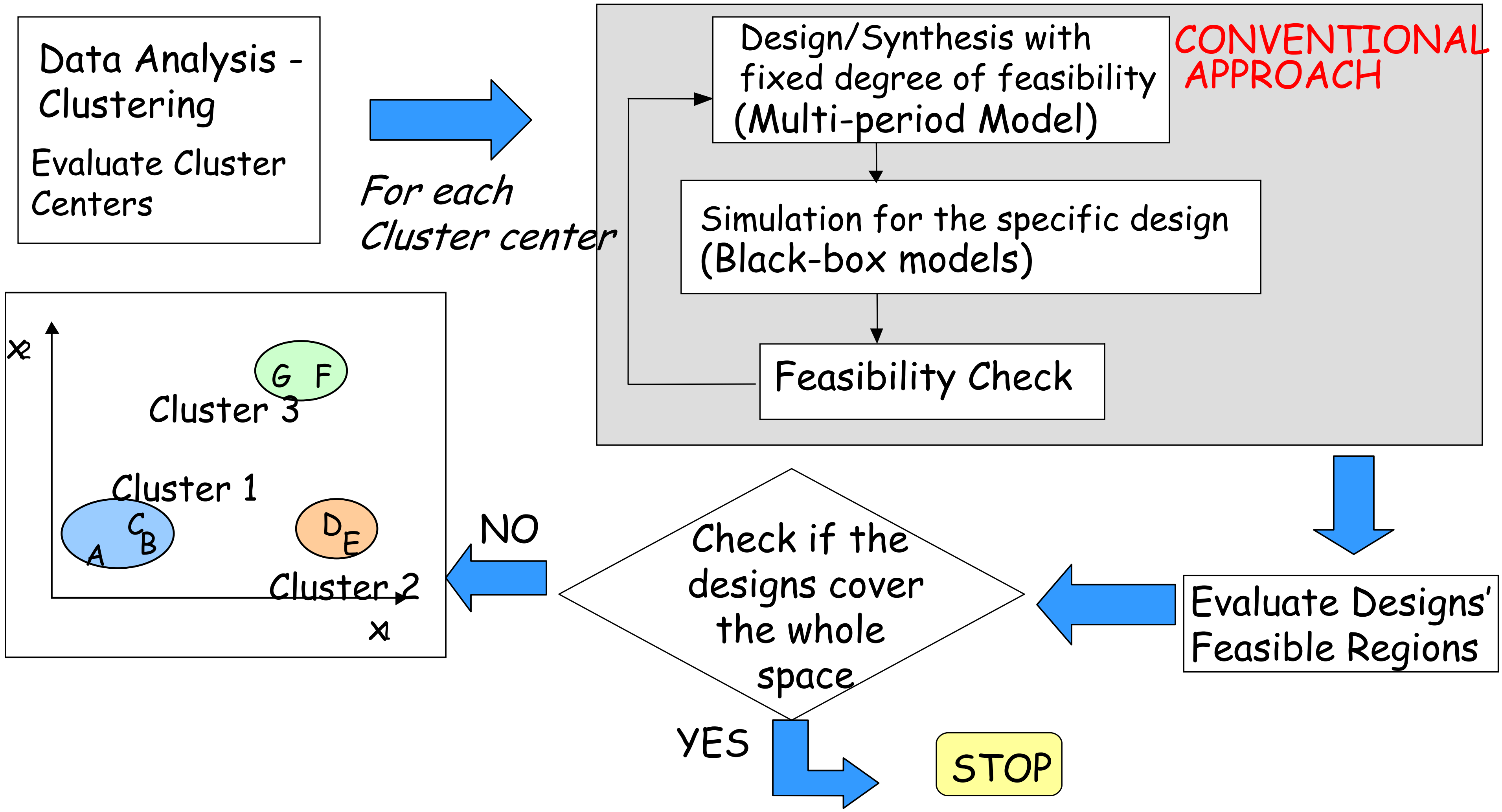
- Find *representative* objects, called medoids, in clusters

- ***PAM*** (Partitioning Around Medoids) starts from an initial set of medoids and iteratively replaces one of the medoids by one of the non-medoids if it improves the total distance of the resulting clustering.

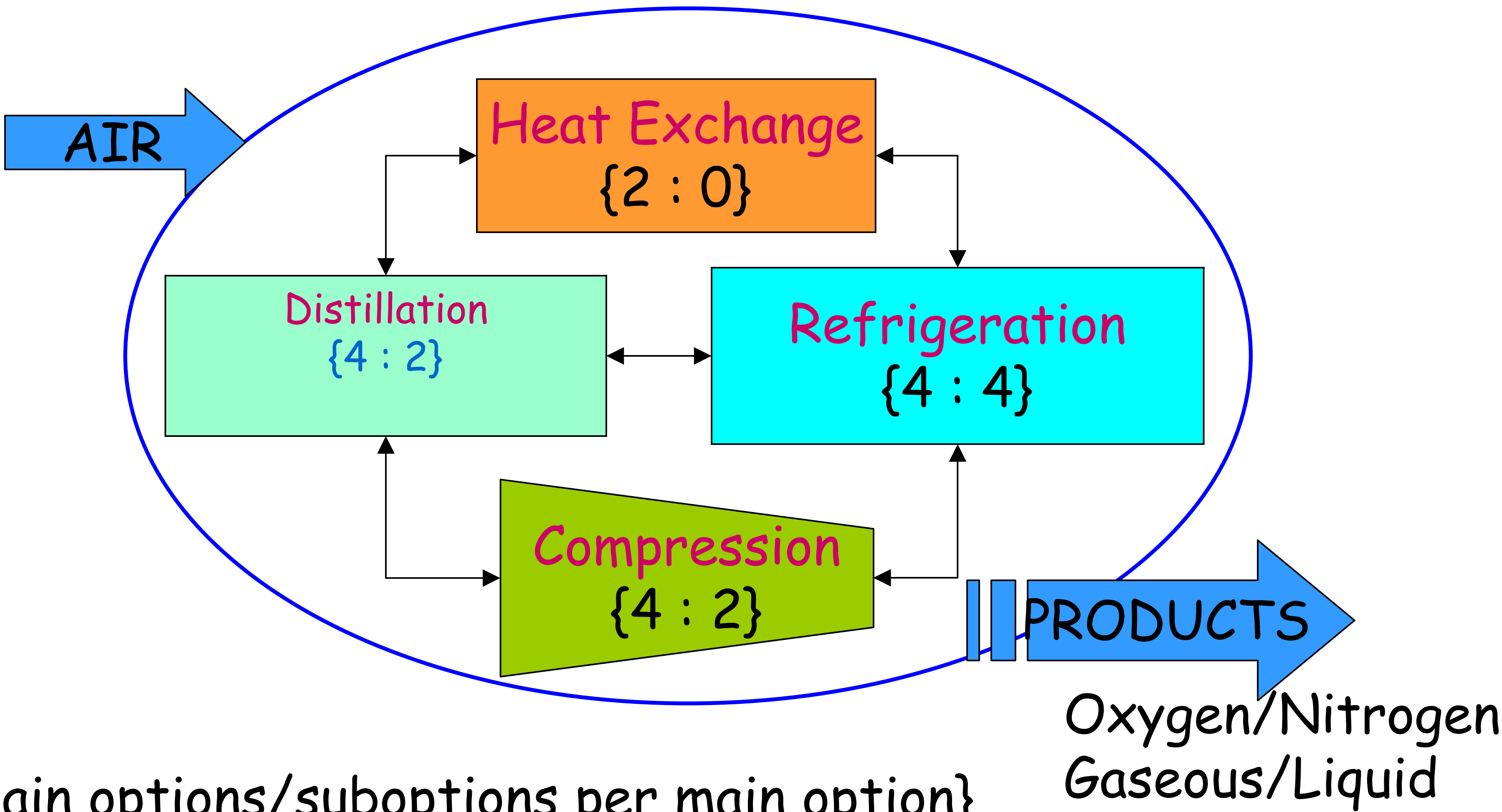
Kaufman and Rousseeuw, Finding Groups In Data (1990)

Design Optimization Integrating Market data

Integration with Design Optimization



Air Separation Plant Superstructure



{main options/suboptions per main option}

Air Separation Case Study:Sample Demand Source

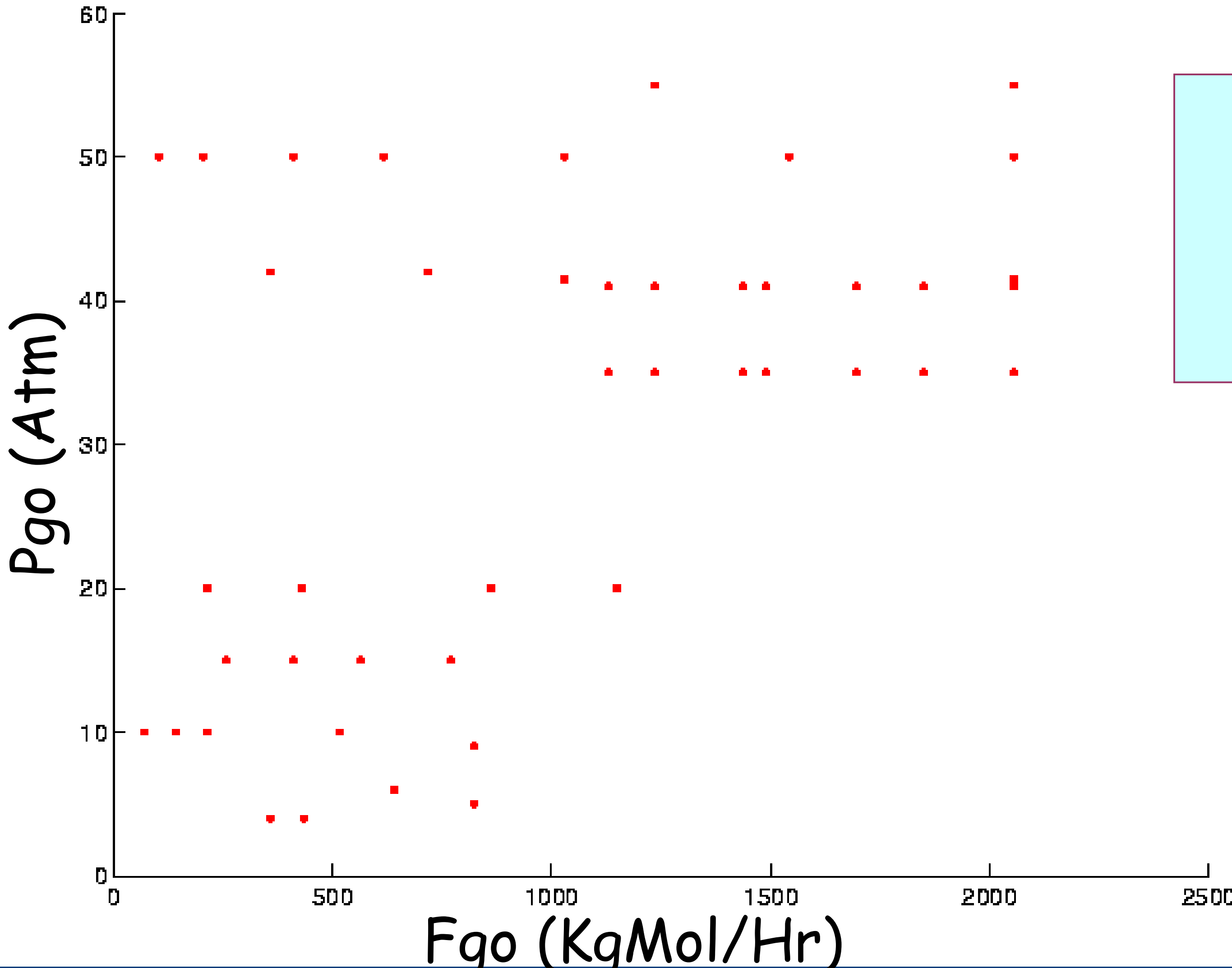
Factors for Consumption of Oxygen (tons per ton of product)

Product	Consumption
Ethylene Oxide	1.01
Propylene Oxide	1.26

Sample Plant Capacities (million lb/yr)

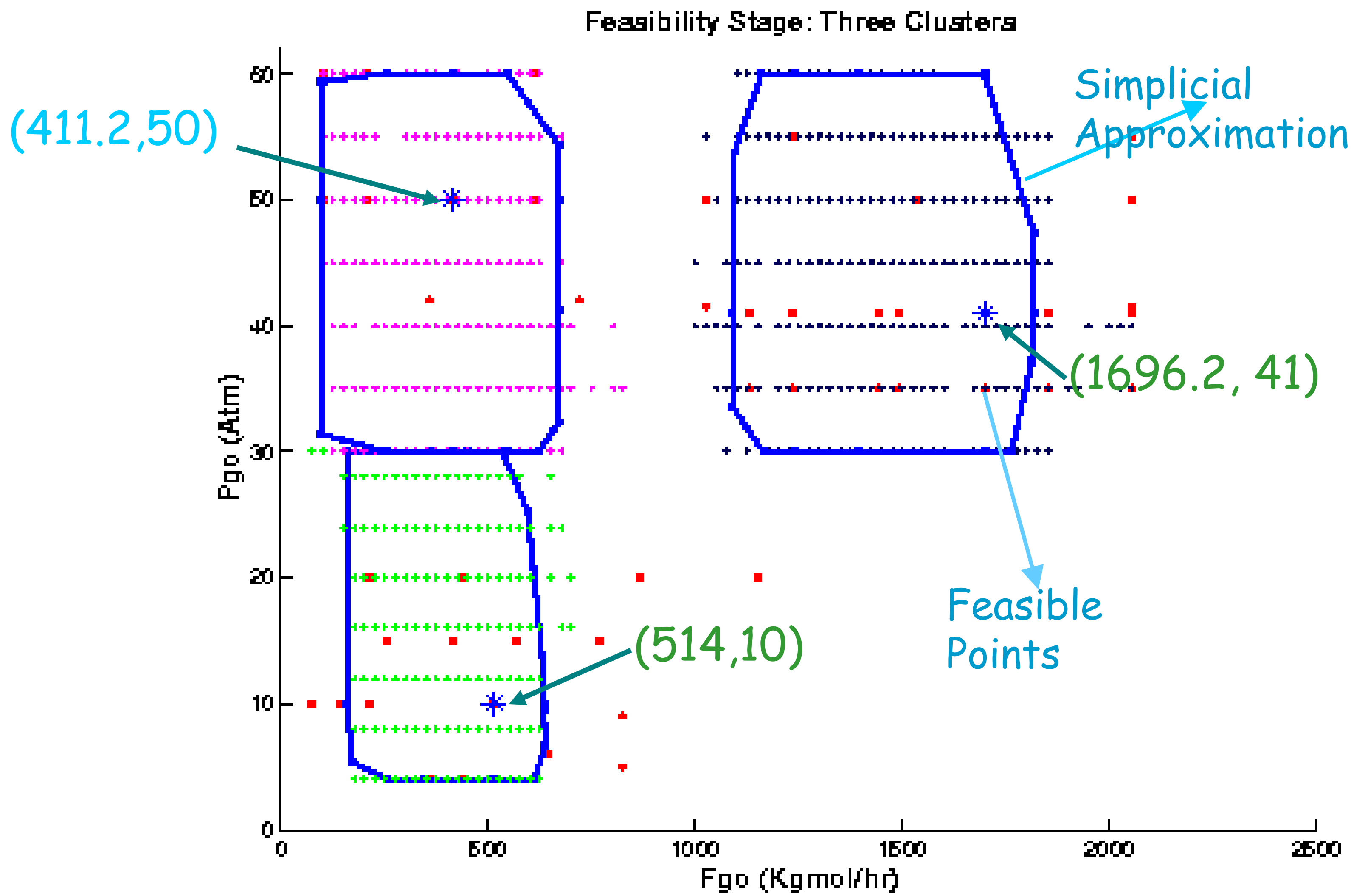
Ethylene Oxide	150	300	600
Propylene Oxide	200	400	800

Demand Data

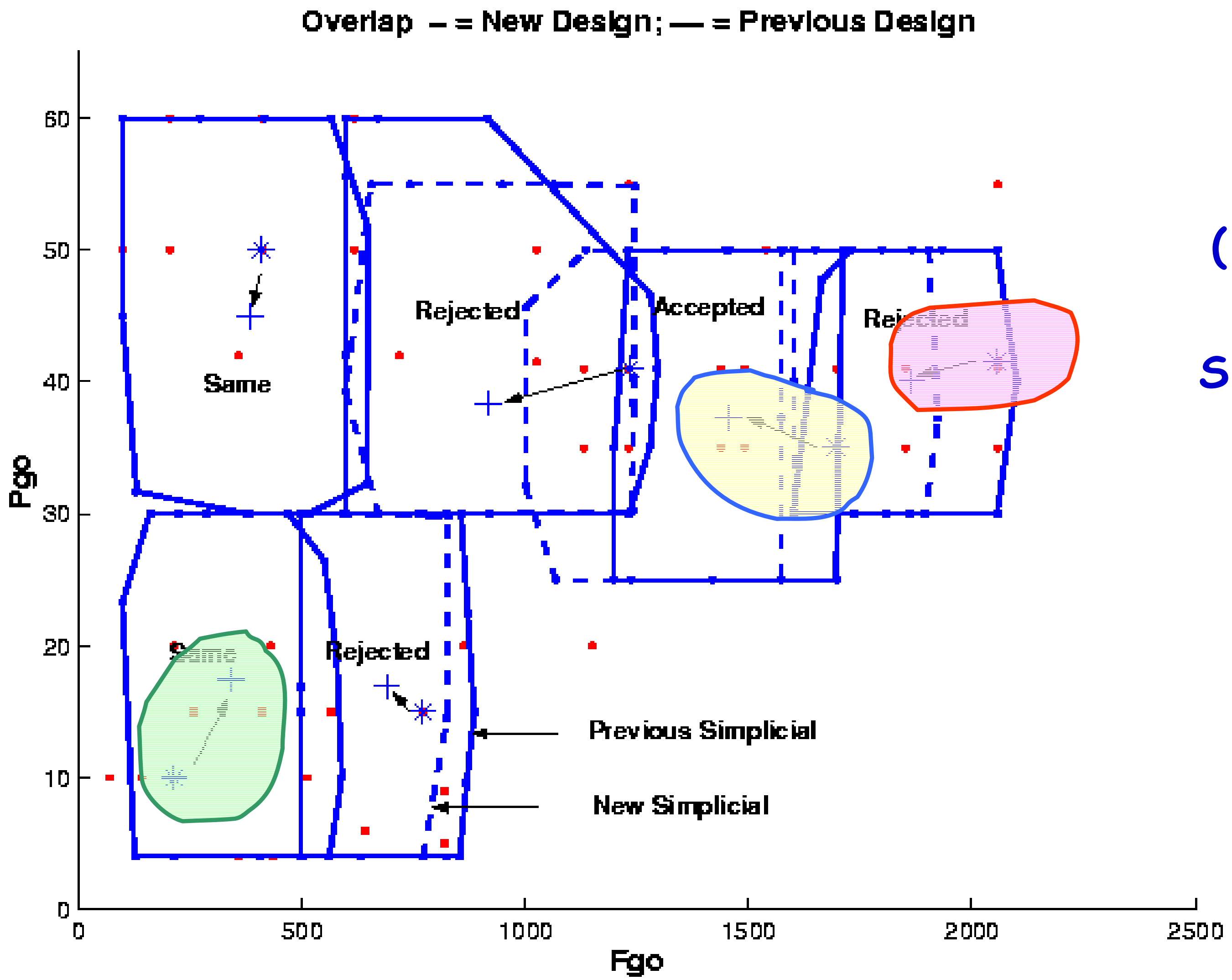


Each point represents a different potential customer

Results – Iteration 1 (3 Clusters)



Optimality Stage



(1696.2, 35)

(1455.4, 37.25)

Lower Cost

Similar Flexibility

Accepted

(2056, 41.5)

(1867.5, 40)

Lower Cost

Lower Flexibility

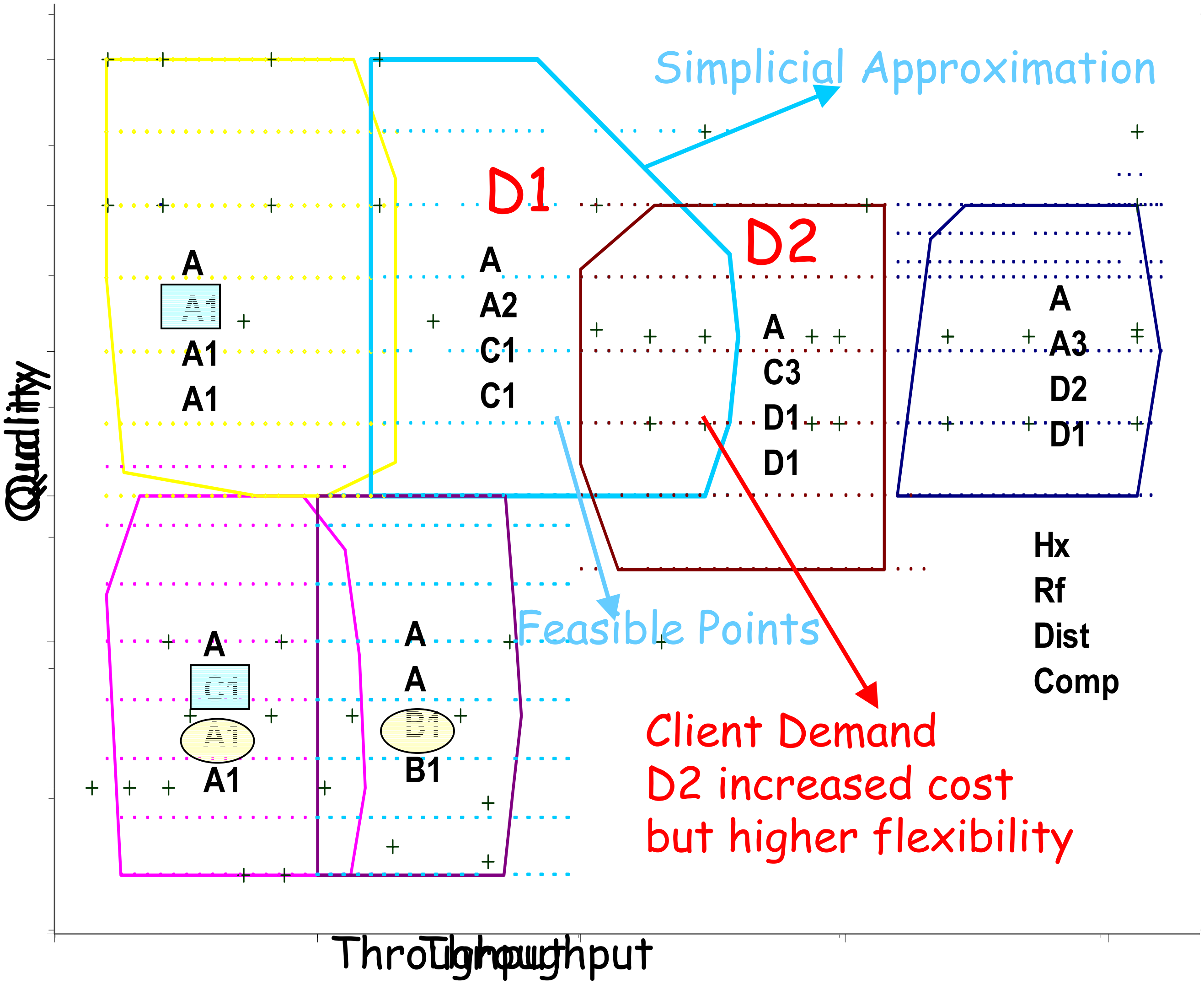
Rejected

(215.9, 10)

(343.7, 17.4)

SAME

Final Design Portfolio



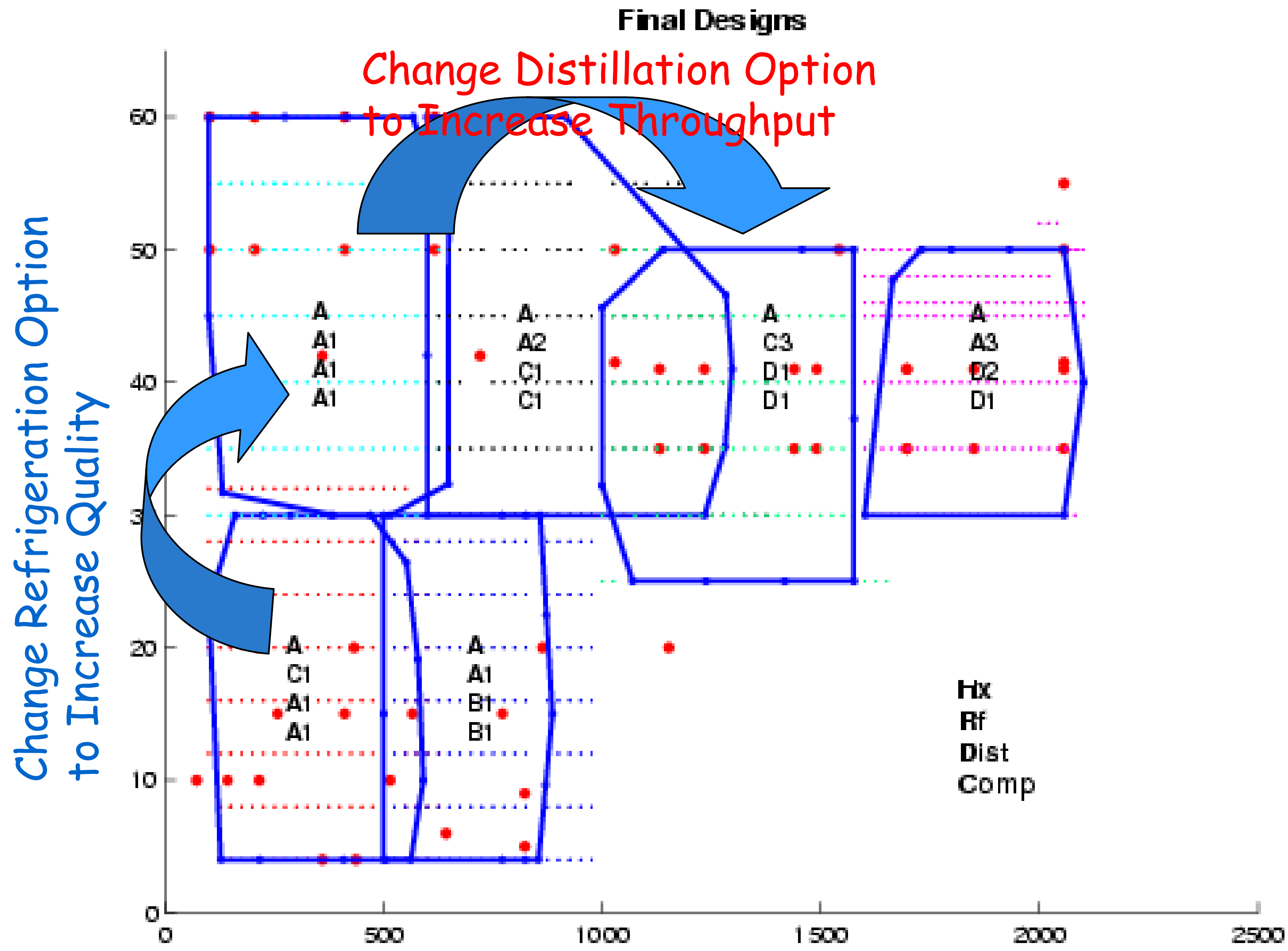
Multiple Clients

Accurate descriptio of the operability boundaries

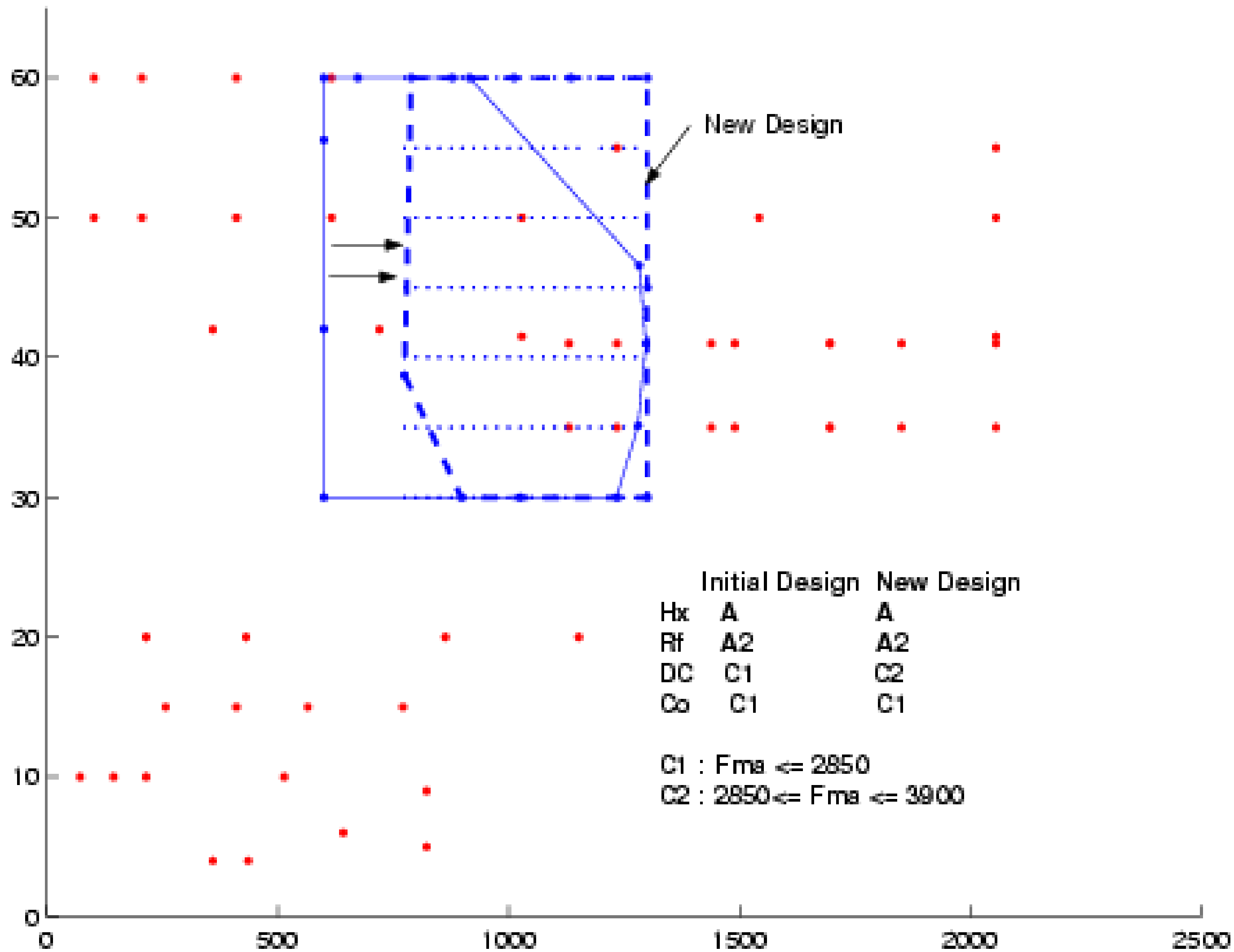
Trade-offs betweer cost and flexibility

Sensitivity to differ units

Sensitivity to Different Units



Introduction of New Technology

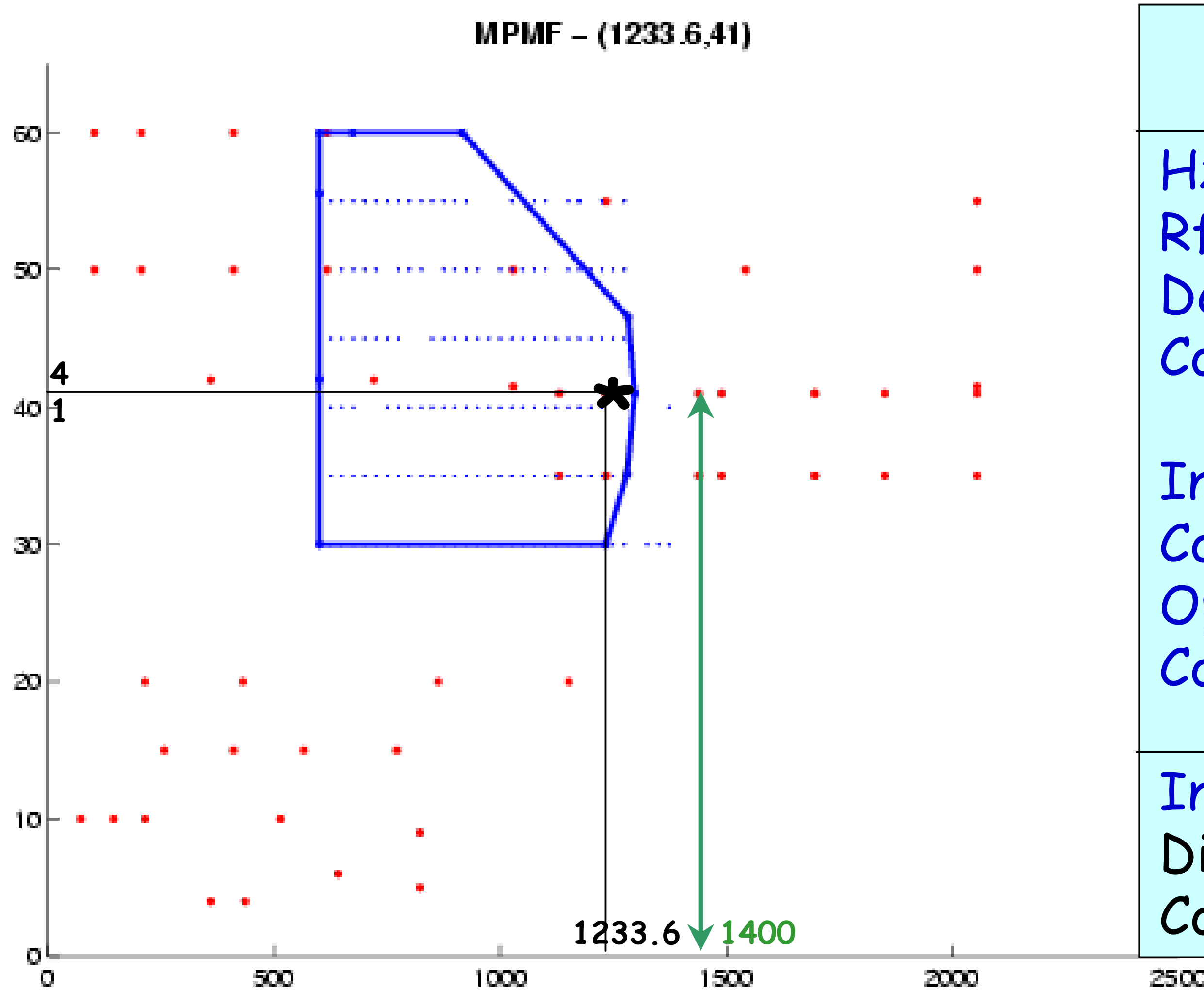


Changing Compressor to Larger Capacity

DOES NOT

Increase Plant Flexibility

Staging Design - Spare Units



	Initial Design	New Design
Hx	A	A
Rf	A2	A2
Dc	C1	C1+A1
Co	C1	C1+A1
Inst. Cost	13E6	20.18E6
Oper. Cost	11.E6	12.8E6

Incremental Cost:
Distillation: 2.1E6
Compressor: 5.07E6

Relevance and Importance

Manufacturer: Modular-based designs are substantially cheaper than customized designs and can satisfy larger range of demands

Customer: Greater flexibility in decision making at design stage as different design alternatives can be considered based on expected demand and economic feasibility

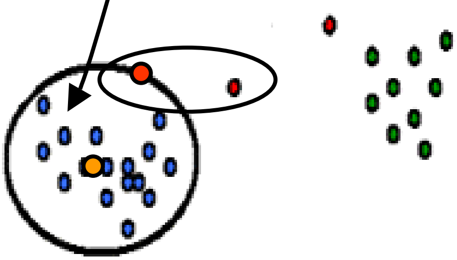
Multi-Period Robust Design Optimization

Min $\sum_i$ Capital and Operating Cost

Robustness Cost

$+$ $\lambda \sum_i$ (variance in operating cost)^2 $\qquad \lambda \sum_{i=1}^{n} w^i (C^i - \sum_{i'} w^i C^{i'})^2$

$+$ $\beta \sum_i$ (Un-met Demands)^2 $\qquad \beta \sum_{j=1}^{m} \sum_{i=1}^{n} w^i (z_j^i)^2$



Subject to:

- Process Constraints

$$\mathbf{h}(d, x^i, u^i, \theta^i) = 0 \qquad \forall i$$

$$\mathbf{g}(d, x^i, u^i, \theta^i) \le 0 \qquad \forall i$$

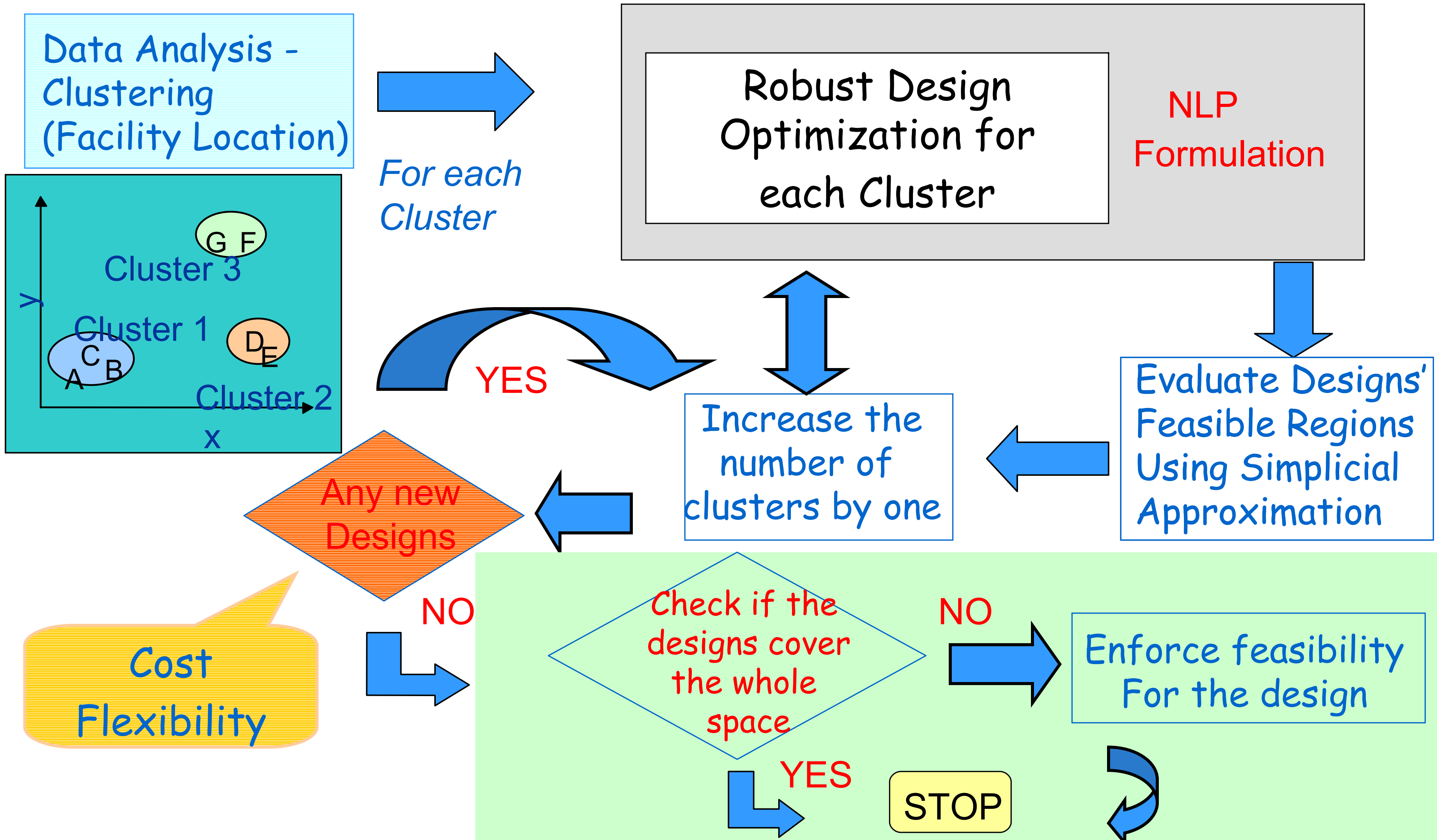
- Un-met Demand Constraints

$$F^i_{Prod\_j} + \mathbf{z}^i_j \ge F^i_{demand\_j} \qquad \forall i, j$$

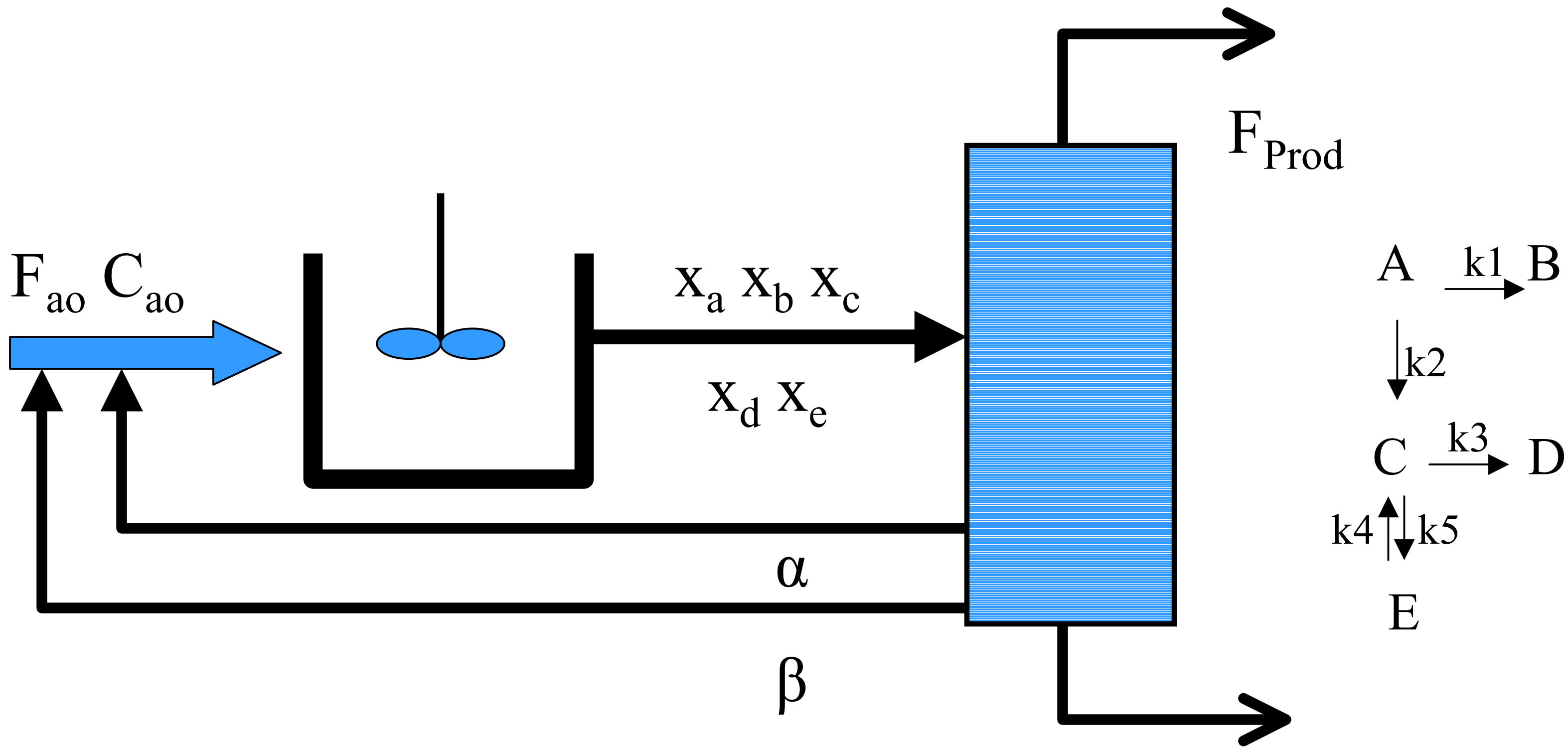
i = periods, λ, β = robustness parameters

*Mulvey et al., Robust Optimization of Large Scale Systems, Oper. Res., 1995

Flexible Module-Based Design Generation

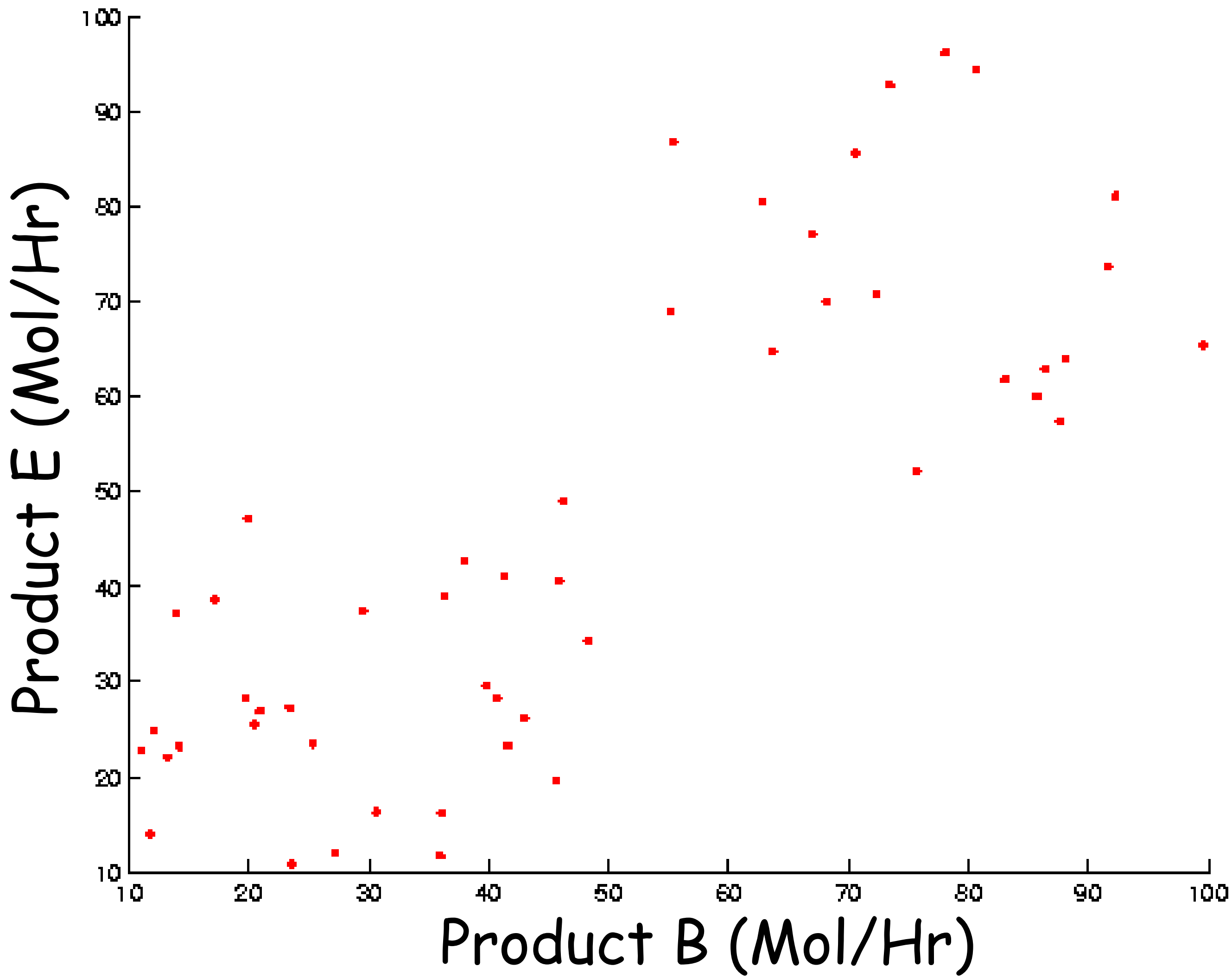


Illustrating Case Study

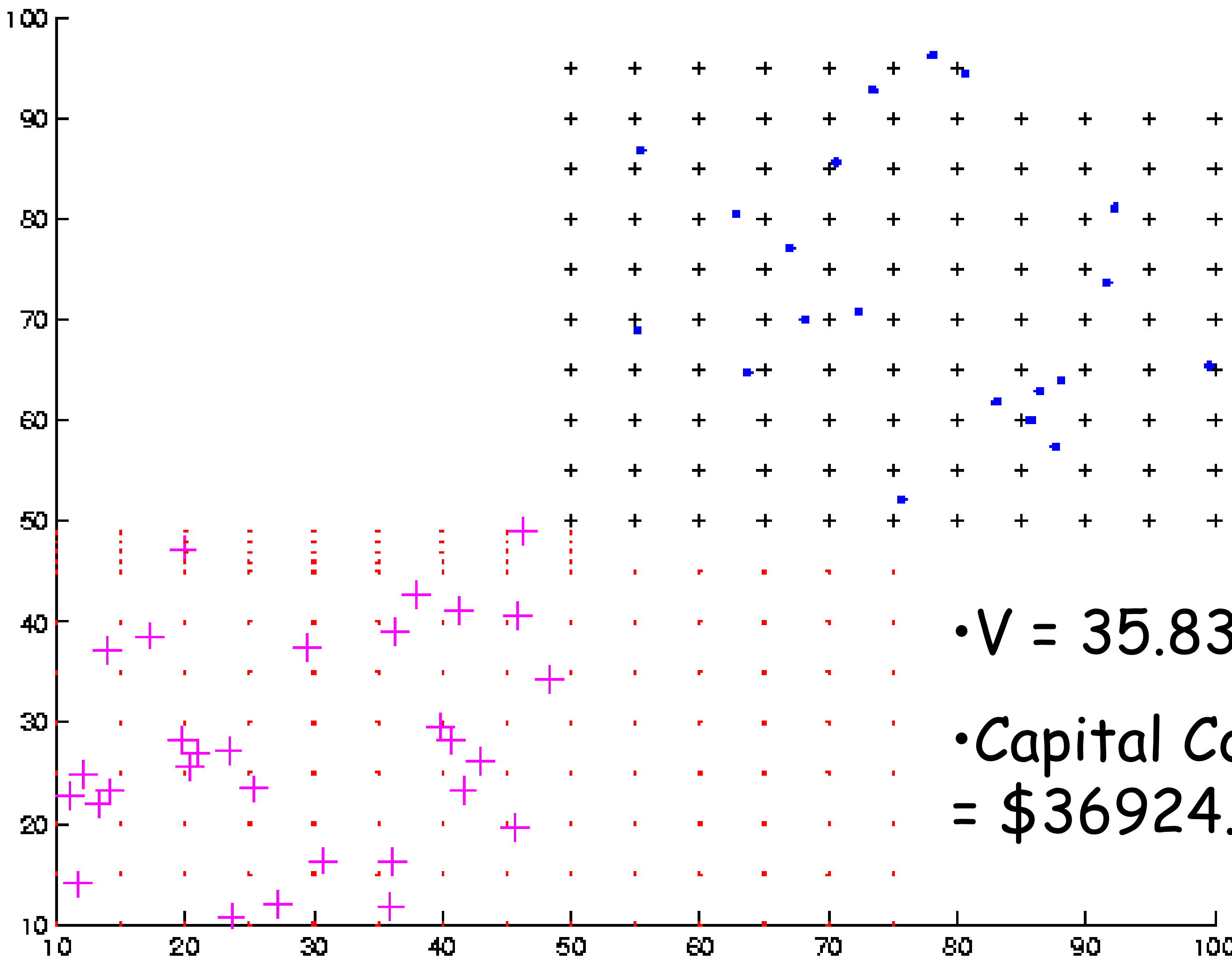


- Given rate-constants and demand
- Determine CSTR Volume, Input F_{ao} and C_{ao} that minimize overall cost

Demand Data



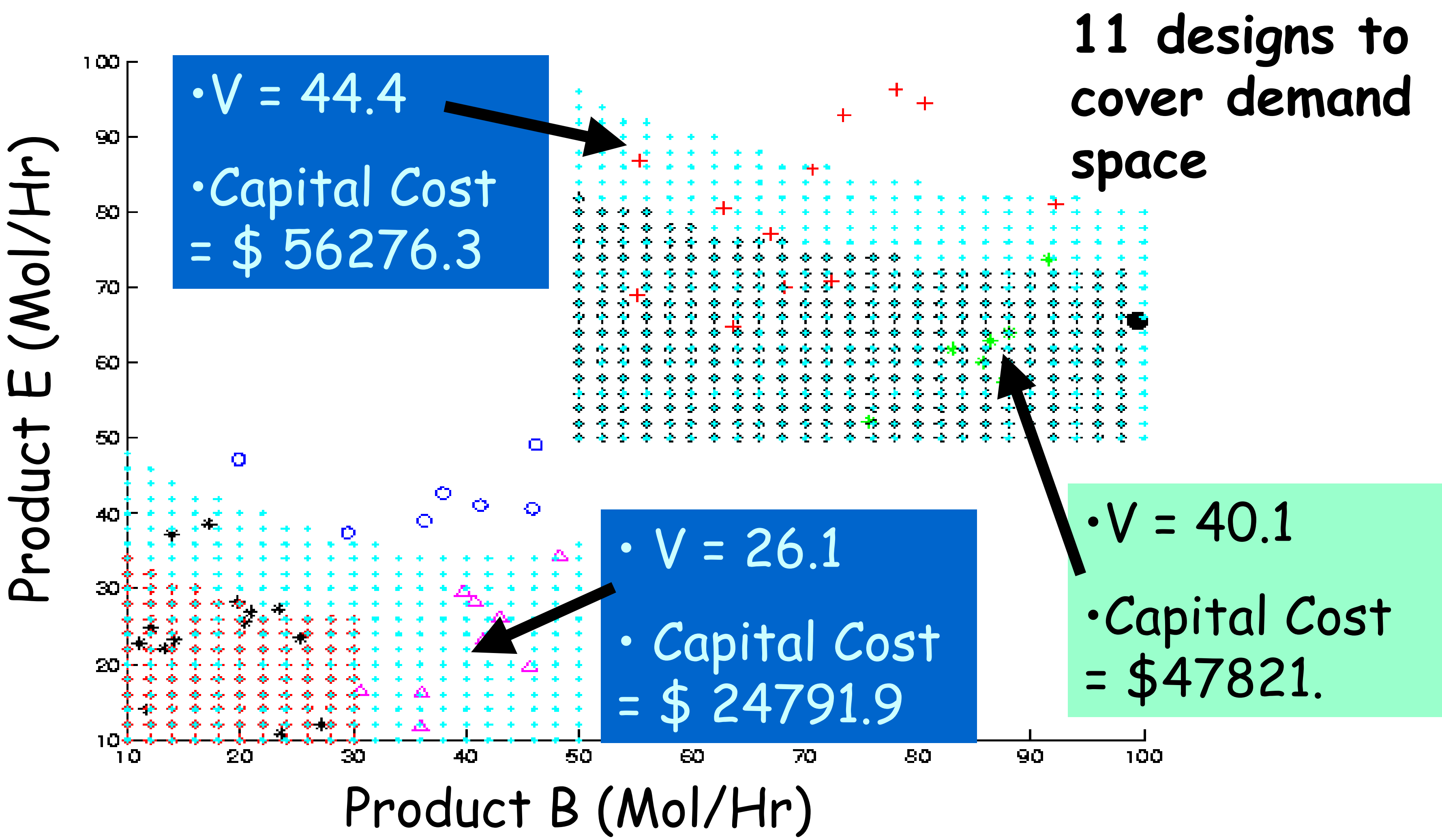
Results – Iteration 1 (2 Clusters)



- V = 49.17
- Capital Cost = $67006.7

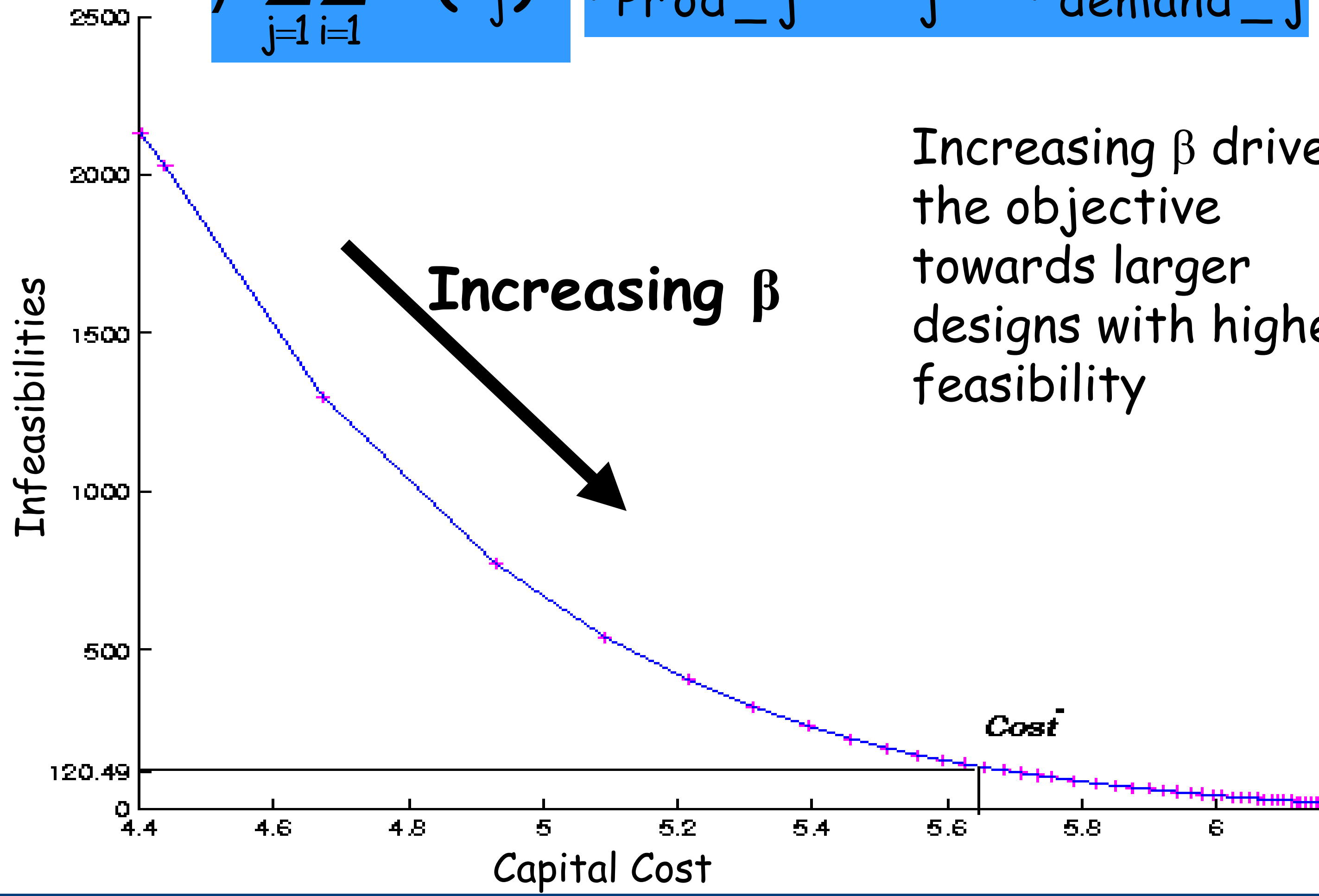
- V = 35.83
- Capital Cost = $36924.6

Iteration 4 (5 Clusters)



Capital Cost vs Feasibility

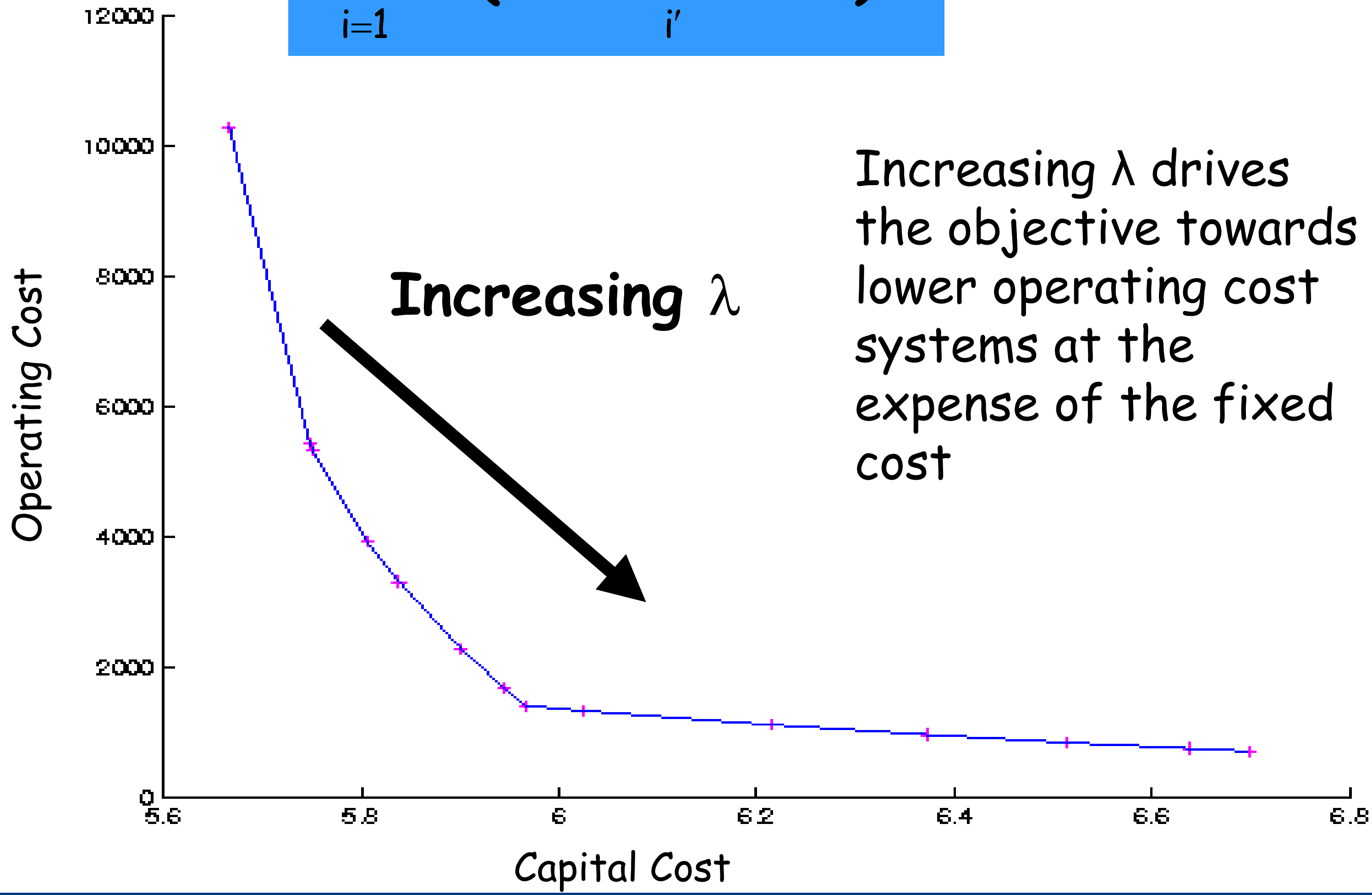
$$\beta \sum_{j=1}^{m} \sum_{i=1}^{n} w^i (z^i_j)^2 \qquad F^i_{Prod\_j} + \mathbf{z}^i_j \geq F^i_{demand\_j}$$



Increasing β drives the objective towards larger designs with higher feasibility

Capital Cost vs Robustness

$$\lambda \sum_{i=1}^{n} w^i \left(C^i - \sum_{i'} w^i C^{i'} \right)^2 -$$



Increasing λ drives the objective towards lower operating cost systems at the expense of the fixed cost

Optimization of Noisy Systems

Optimization of Noisy Functions

- *Programming Model*:*

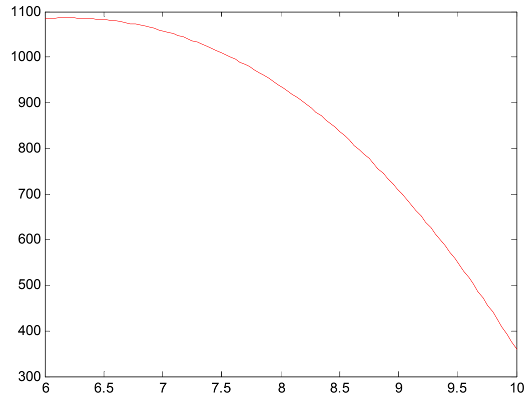
$$\min \; Z = c^T y + F(x,\varepsilon)$$

$$\text{s.t.} \quad h(X) = 0$$

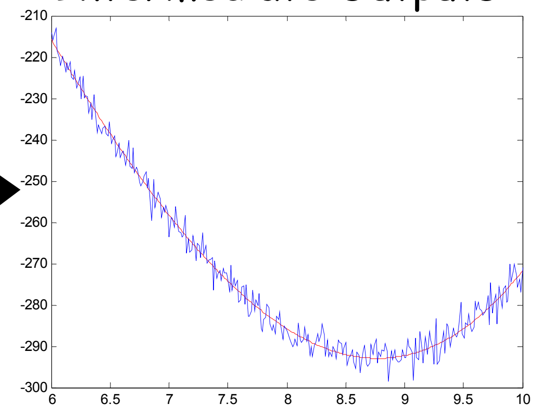
$$g(X) + My \leq 0$$

$$x \in X, y \in Y$$

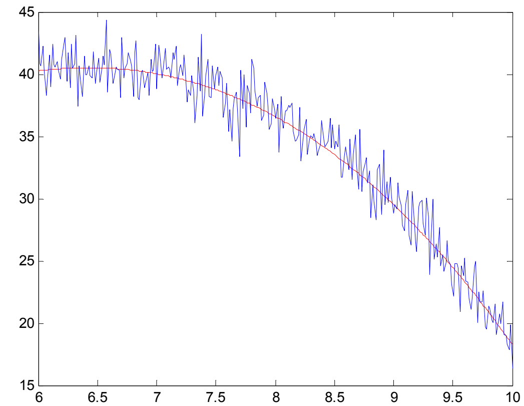
Inputs x



Intermediate Outputs



Final Outputs

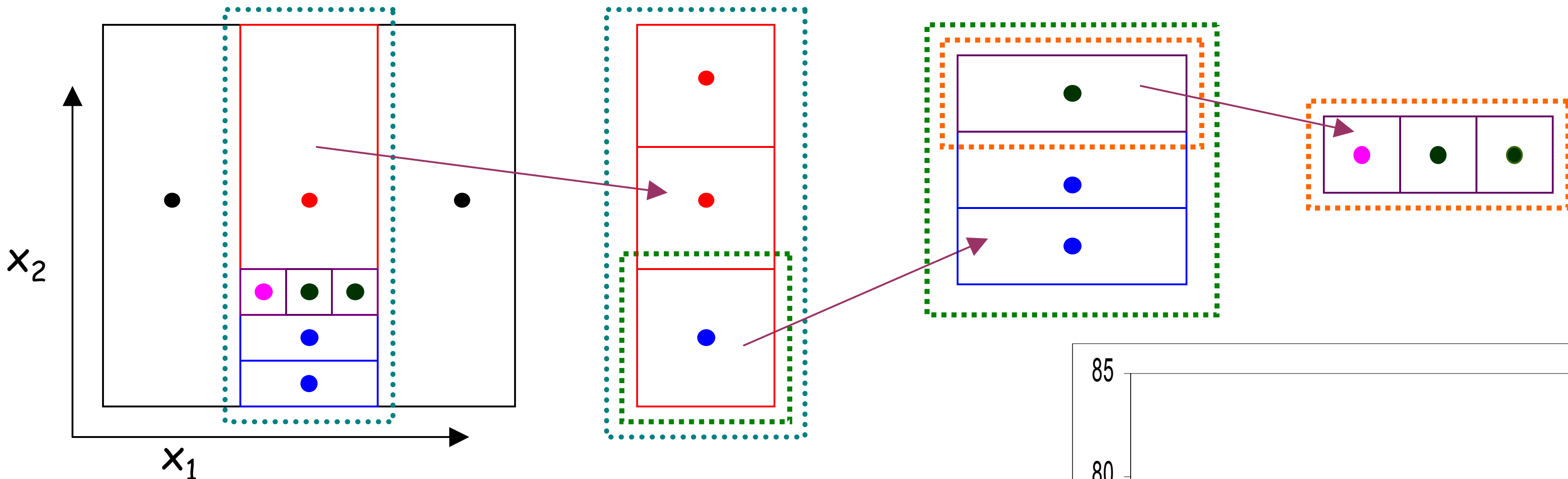


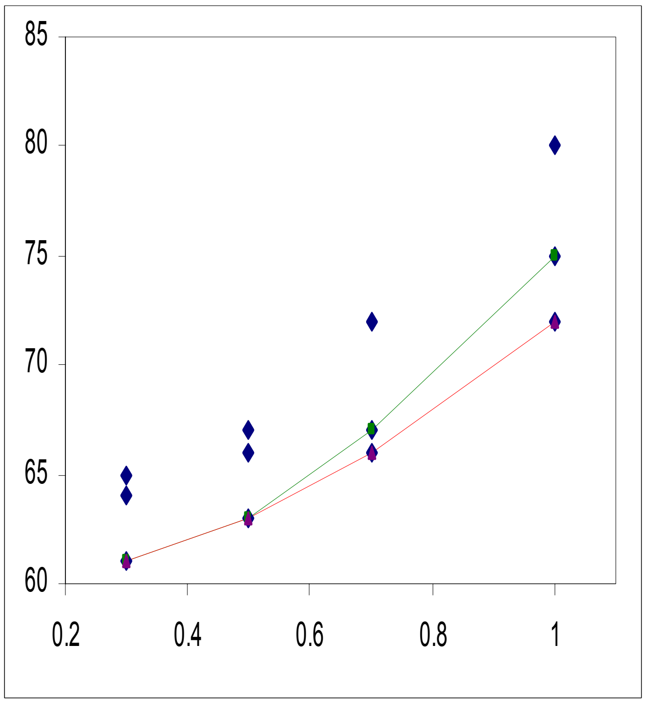
- X is a vector of continuous variables, (P, T, Flowrates)
- Y is a vector of binary variables, (existence of a particular stream or unit)
- The uncertainty ε can propagate or dampen as the process moves forward
- Optimality conditions cannot be defined at optima
- Conventional algorithms may become trapped in artificial local optima or even fail completely

*Biegler et. al., Systematic Methods of Chemical Process Design, (1997), 513

Existing Work

DIRECT "DIvided RECTangles in action" (Jones et. al., 1993)





•Splits feasible region into hyper-rectangles and samples at center points → global search

•Scatter plot created to discover which sample points lie below a prescribed improvement in the objective → local search

•If the best point is unsatisfactory, smaller hyper-rectangles are inscribed inside region and sampling at the centers of these new regions continues

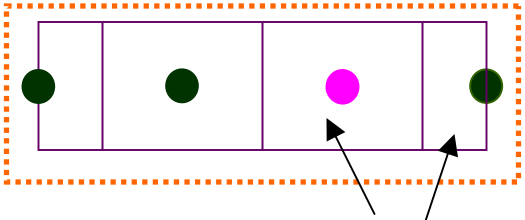
•Slow to converge, especially if the optimum is along a boundary

Existing Work

Multilevel Coordinate Search (Huyer & Neumaier, 1998)

•Avoids slow convergence of DIRECT by sampling at boundary points

•Newton-based methods/SQP minimize interpolating polynomials to obtain new regions for sample points

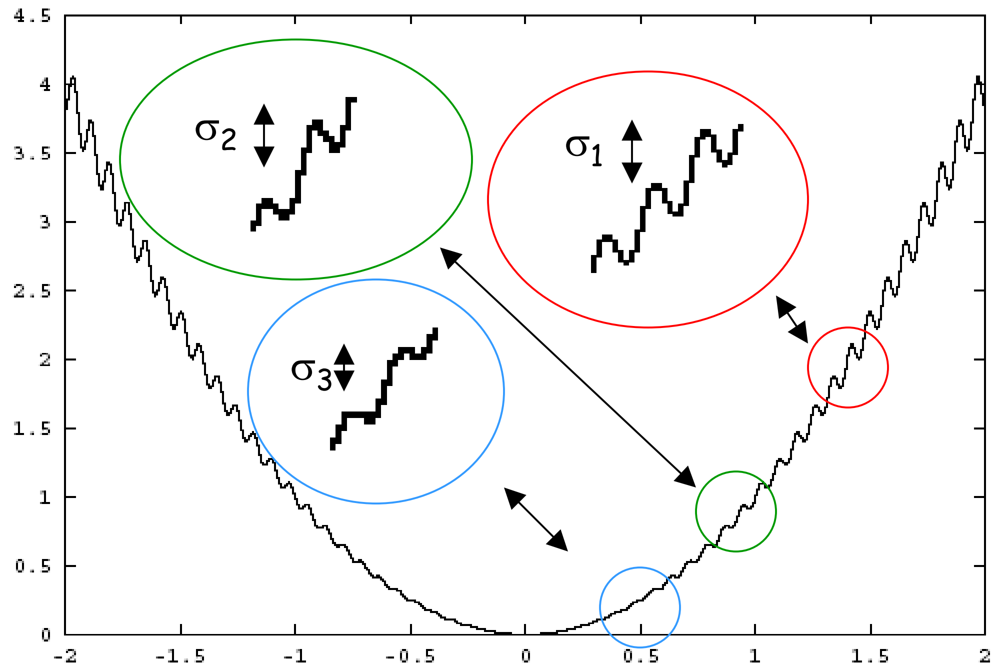


Irregularly split regions allow larger area to be sampled during local search

Implicit Filtering (Choi & Kelley, 1999, Gilmore & Kelley, 1994)

•Applies Newton-based methods with step sizes proportional to high-frequency noise, "filtering", or "stepping over" low-frequency noise

•Successively decreases the step size as optimum is approached



Existing Work

Differential Evolution (Storn & Price, 1995)

$X_{i,G} = [X_{i1,G}\ X_{i2,G} \ldots X_{iD,G}]$

Gen. G

$X_{1,G}$

$X_{2,G}$

:

:

$X_{N,G}$

Choose multiplier $F \in [0,2]$

For i = 1…N:

Randomly select integers

$r_1, r_2, r_3 \in 1\ldots N,\ r_a \neq r_b \neq i$

$V_{i,G} = X_{r1,G} + F(X_{r2,G} - X_{r3,G})$

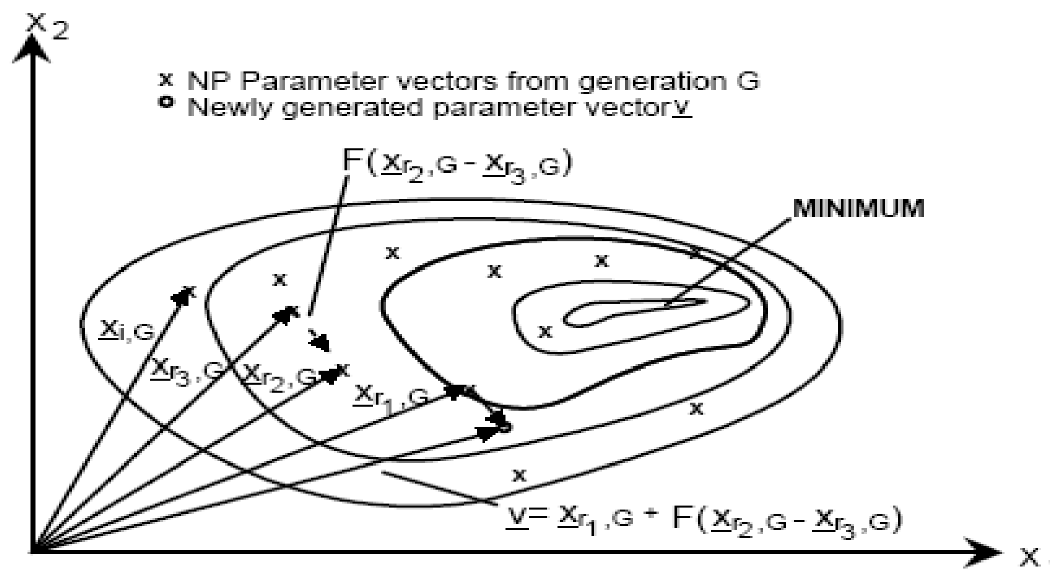
Select crossover index $CR \in [0,1]$

Select $\Gamma(i)$ = integer $\in 1\ldots D$ (ensures at least one element from $V_{i,G}$ mixes with $X_{i,G}$

$\beta(j) \in U[0,1],\ j = 1\ldots D$

$$X_{ji,G+1} = \begin{cases} v_{ji,G} \text{ if } (\beta(j) \leq CR) \text{ or } (j = \Gamma(i)) \\ x_{ji,G} \text{ if } (\beta(j) > CR) \text{ and } (j \neq \Gamma(i)) \end{cases}$$

$X_{1,G}$	+	$V_{1,G}$	→	$X_{1,G+1}$
X_{11}		V_{11}		V_{11}
X_{12}		V_{12}		X_{12}
X_{13}		V_{13}		V_{13}
X_{14}		V_{14}		X_{14}
X_{15}		V_{15}		X_{15}
X_{16}		V_{16}		V_{16}



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Existing Work

Determination of Optimal Step Sizes for Finite Differences (Brekelmans et al., 2003)

- F(x) is unknown → How to obtain gradient information for optimization?
- Assume E(ε) = 0, Var(ε) = σ^2 (ε independent of x) → model F(x,ε) as g(x) = F(x) + ε
- Estimate of forward finite difference (example): $\boldsymbol{\beta}^{FFD}(h) = \dfrac{g(x+h)-g(x)}{h}, h > 0$
- Applies statistical arguments to Taylor series expansions of F(x) to determine:

$$E\left(\left\|error_s^{FFD}\right\|^2\right)$$

$$Var\left(\left\|error_s^{FFD}\right\|^2\right)$$

$$Var\left(\left\|\beta^{FFD}(h) - \nabla f(x)\right\|\right)$$

where

$$error_d^{FFD} = \left(\frac{f(x+h)-f(x)}{h}\right) - \nabla f(x)$$

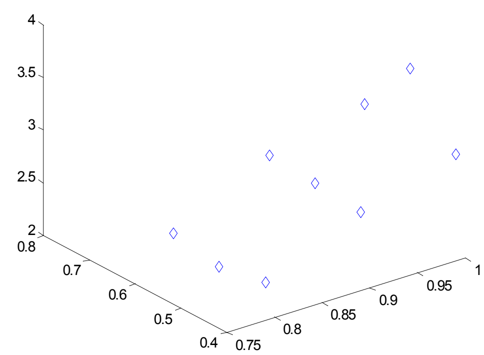
$$error_s^{FFD} = \left(\frac{\varepsilon(x+h)-\varepsilon(x)}{h}\right)$$

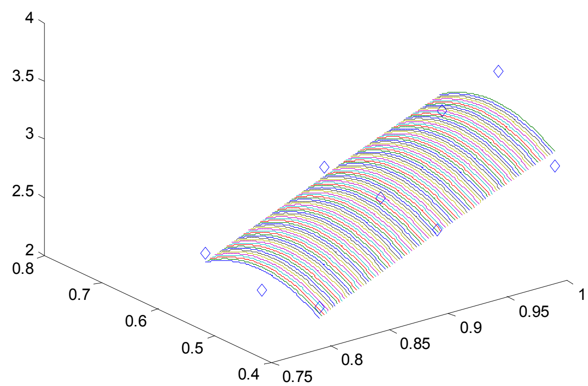
Unknown

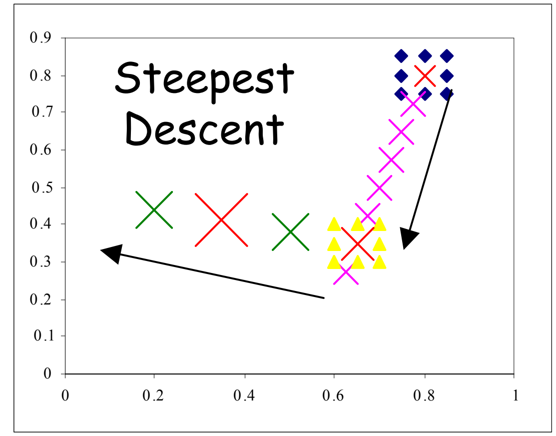
- Provides bounds on convergence – upper limit on the stochastic error and the maximum variance of the difference in the estimated and true gradient
- Expressions obtained for forward/backward/centered finite differences, as well as for Plackett-Burman and Factorial Designs
- Requires estimate of the maximal (n+1)th order derivative (e.g. for FFD, need value for the second-order portion of the Taylor series)

Existing Work

Response Surface Methods (Myers/Montgomery, 2002, Jones, 2001, Jones et. al. 1998)







$$(x_{1,1} \dots x_{1,k}) = f(x_{1,1} \dots x_{1,k})$$

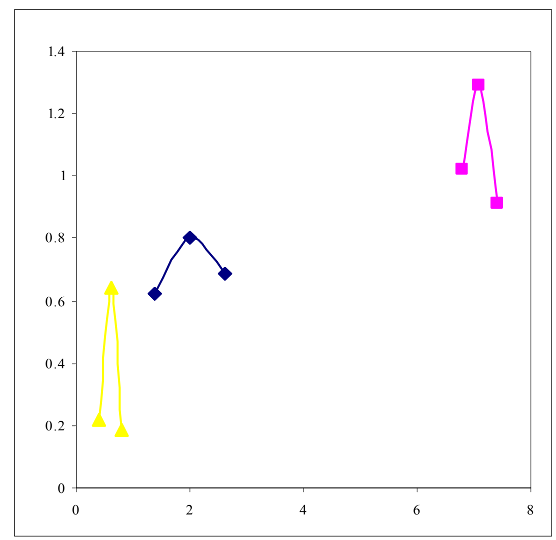
$$\vdots \qquad\qquad \vdots$$

$$(x_{n,1} \dots x_{n,k}) = f(x_{n,1} \dots x_{n,k})$$

$$\left\{ \begin{array}{l} A = \sum_{i=1}^{n} c_i B_i(x_{i,1} \dots x_{i,k}) \\ A = \sum_{i=1}^{n} \lambda_i \, \varphi\left(\left\| X - X_i \right\|\right) + c_i B_i(X) \end{array} \right\}$$

Radial Basis Functions (Gaussian-type functions) "correctors" to basis functions B_i for fitting scattered data groups

$$\sum_{j=1}^{k} \frac{dA}{dx_j} = 0 \quad \Rightarrow \quad (x_1 \dots x_k)^{opt}$$



The Problem

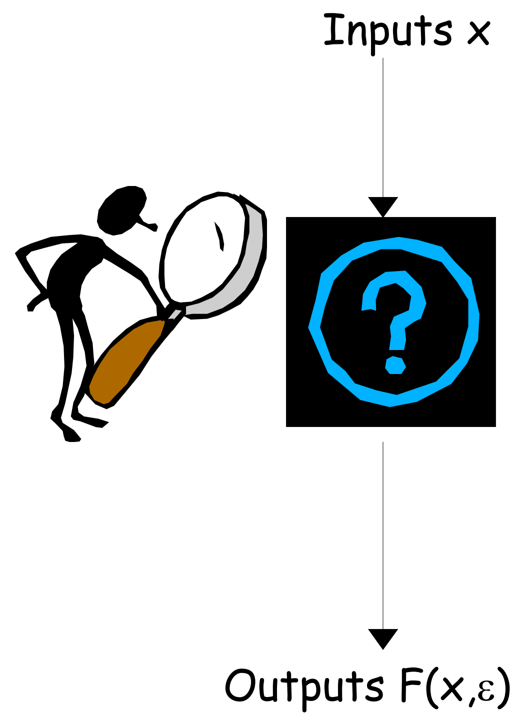
•Given that systems exist where closed-form equation models are not available or inaccurately describe the physical and chemical behavior,

•Given that processes of interest are moving to a smaller and smaller scale, in which model equations may be unknown,

•Given that process noise is expected to be present regardless of the system scale (macro, micro, nano),

•Given that conventional optimization algorithms can fail for noisy systems due to becoming trapped in artificial local optima, thus terminating prematurely,

•How can we optimize stochastic systems where closed-form equation models are inaccurate or nonexistent – i.e. optimize “black-box” models?



- Stochastic input-output data are the only reliable information available for optimization

- Model development is complicated since important variables are not known *a priori*

Microscopic Model Example

•Problem: Without knowledge of rate equations, and assuming outputs are noisy, determine (C_A^0, C_C^0) such that $g(C_C, C_D)^{SS}$ is minimized.

$$\min\; g(x,y) = 4(x-0.6)^2 + 4(y-0.4)^2 + \sin^3(\pi x) + 0.4$$

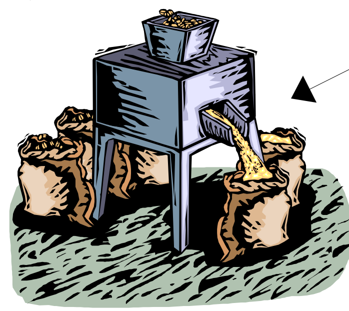
$$\text{s.t.}\quad x = 0.1428 C_C^{SS} - 0.357 C_C^{SS}$$

$$y = -0.1428 C_C^{SS} + 2.857 C_D^{SS} - 1.0$$

$$3 \le C_A \le 30$$

$$0 \le C_C \le 10$$

C_A^0, C_C^0



$A \rightarrow E$

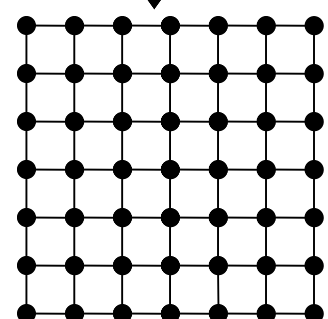
$A \rightarrow D$

$B \leftrightarrow D$

$C \leftrightarrow 2D$

$2A \rightarrow C$

Approximate microscopic process using lattice of size N



$\{C_j(t) + \varepsilon \mid j = A \dots E\}$

Obtaining Computational Model

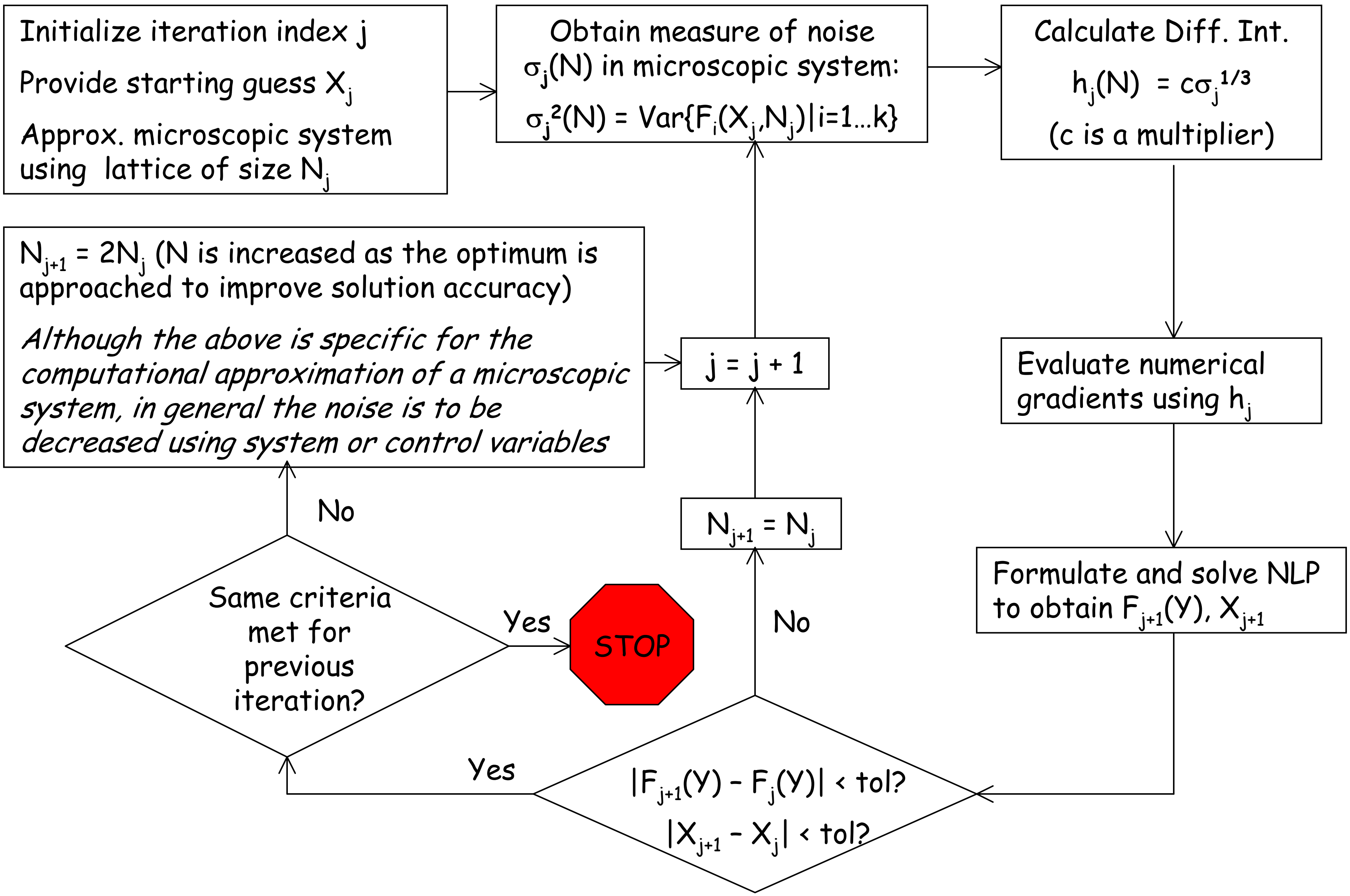
Macroscopic Concentrations $\{C_A, C_C \mid t = 0\}$
→ MS (Initial), $\{\text{Particles } (A,C) \mid t = 0\}^0$

MS (Initial) → Evolve system using Gillespie algorithm
→ MS (Final), $(\text{Particles } (A \dots E))^{SS}$

MS (Final) $\{\text{Particles } (A..E)\}^{SS}$
→ Macroscopic Concentrations $\{C_A \dots C_E\}^{SS}$ → $g(C_C, C_D)^{SS}$

Optimization Subroutine to obtain new iterate, $\{C_A, C_C\}^{new}$

Adaptive Gradient-Based Method



Optimization Using Response Surfaces

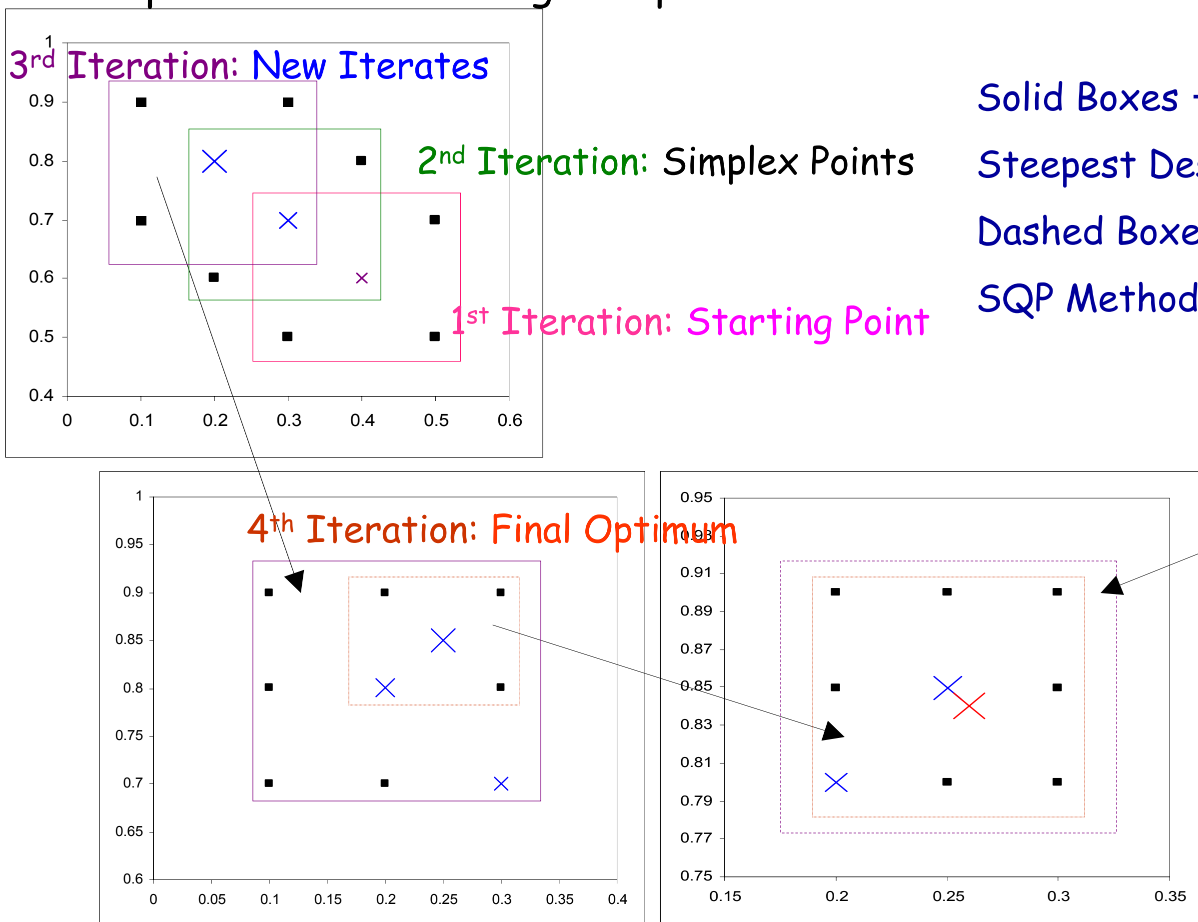
SIMPLEX/STEEPEST DESCENT

Phase I: Move towards optimum using simplices until value in center becomes the winner.

Phase II: Accelerate convergence by optimizing response surfaces using steepest descent

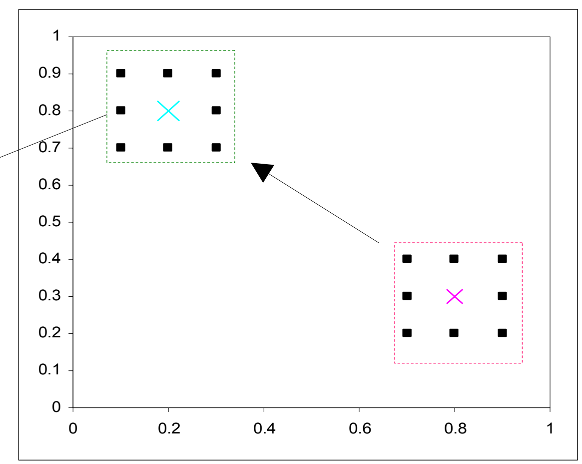
HYBRID RSM / SQP

Create local response surface and formulate quadratic program Solve QP over entire region in order to find next iterate.



Solid Boxes → Local Regions for the Simplex/ Steepest Descent Method

Dashed Boxes →Local Regions for the Hybrid RSM/ SQP Method



Process Operations under Uncertainty

Challenges

Short-term scheduling

- Uncertainty (product prices, demands, etc…)
- Large-scale (large number of units and material flows)

Production Planning

- Longer time horizon under consideration (several months)
- Larger number of materials and products
- Uncertainty in facility availability, product in demand, etc…

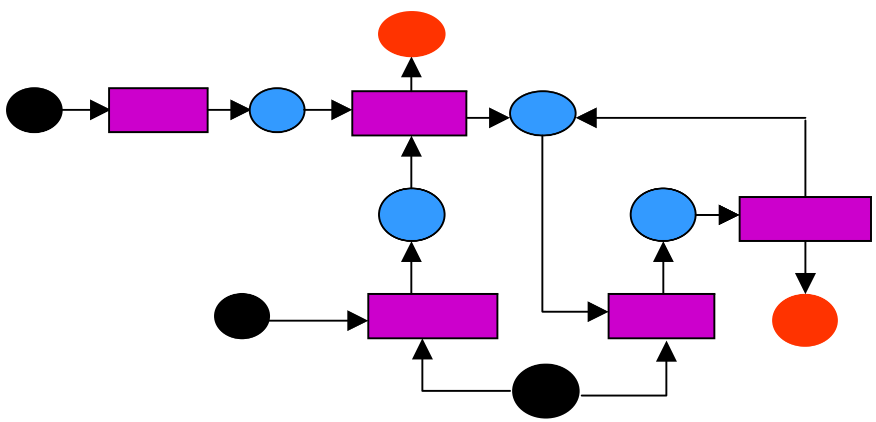
Supply chain management

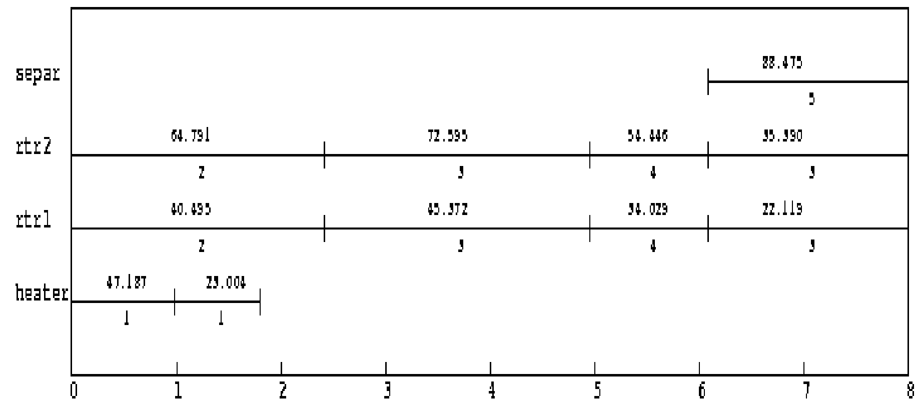
- Multiple sites
  (Involving production, inventory management,transportation etc…)
- Longer planning time horizon (couple of years)

Short-term Scheduling

Process Plant

Optimal Schedule





Given:

Raw Materials, Required Products, Production Recipe, Unit Capacity

Determine:

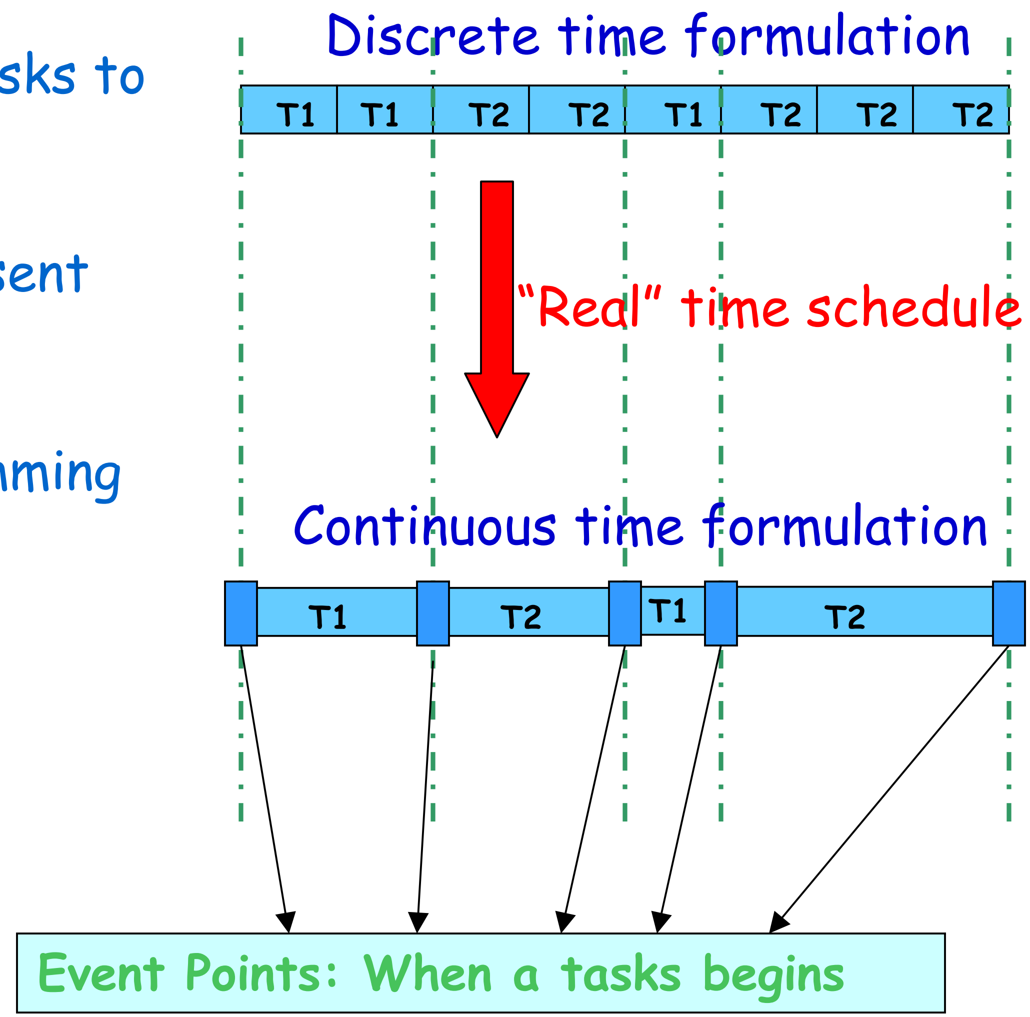
Task Sequence, Exact Amounts of material Processed

Scheduling objectives :

Economic	Maximize Profit, Minimize Operating Costs, Minimize Inventory Costs
Time Based	Minimize Makespan, Minimize Tardiness

Continuous Time Formulation

- Binary variables to allocate tasks to resources
- Continuous variables to represent timing and material variables
- **M**ixed **I**nteger **L**inear **P**rogramming Models
- Smaller models that are computationally efficient and tractable



Deterministic Scheduling Formulation

$$\text{minimize } H \quad \text{or} \quad \text{maximize } \sum_s price(s)d(s,n)$$

Objective Function

$$\text{subject to} \qquad \sum_{(i,j)} wv(i,j,n) \leq 1$$

Allocation Constraints

$$st(s,n) = st(s,n-1) - d(s,n) + \sum \rho^{p} \sum b(i,j,n-1) + \sum \rho^{c} \sum b(i,j,n)$$

Material Balances

$$\left[\begin{array}{c} st(s,n) \leq stmax(s) \\ Vmin(i,j)wv(i,j,n) \leq b(i,j,n) \leq Vmax(i,j)wv(i,j,n) \end{array}\right]$$

Capacity Constraints

$$\sum_n d(s,n) \geq r(s)$$

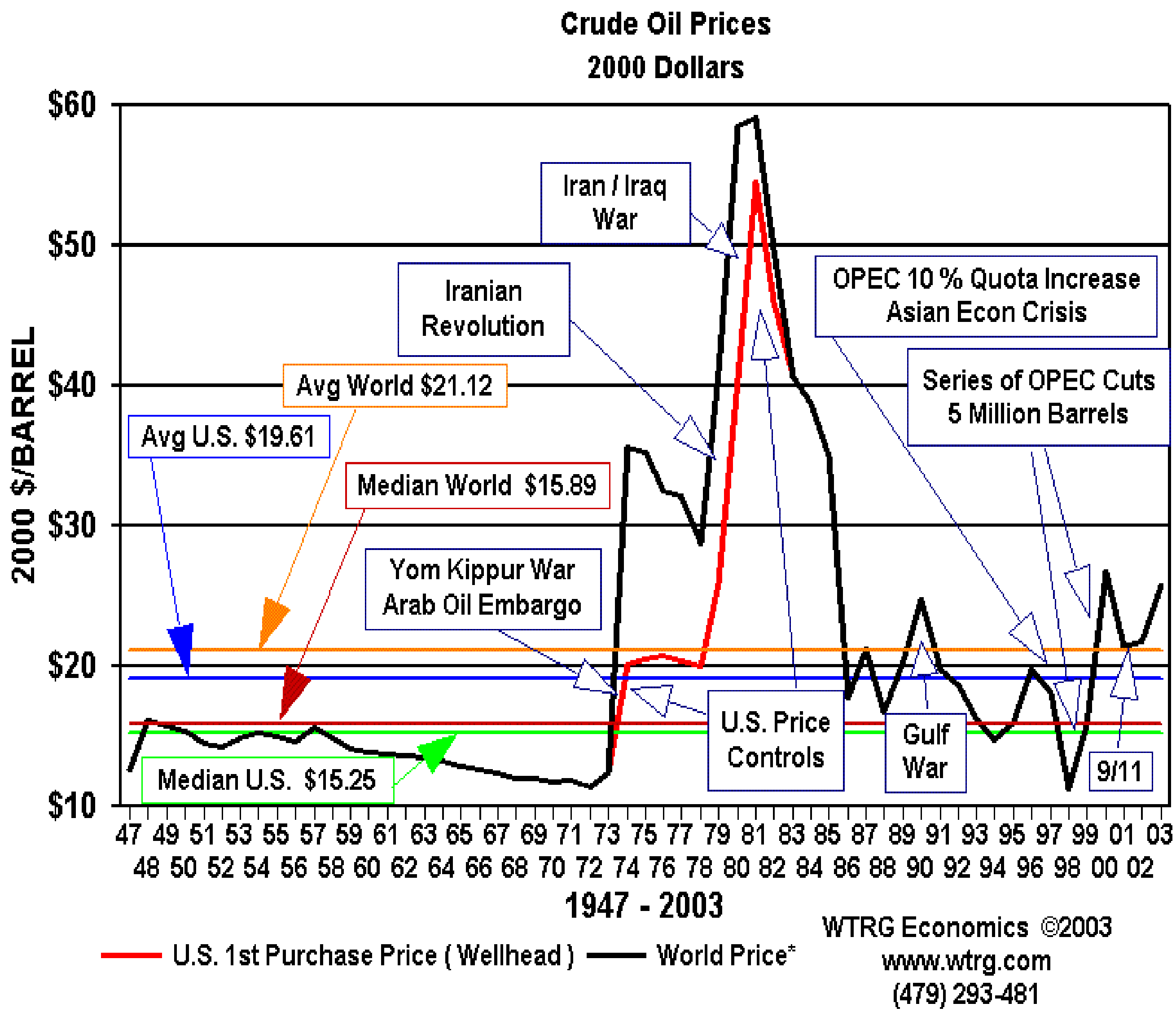
Demand Constraints

$$\left(\begin{array}{c} Tf(i,j,n) = Ts(i,j,n) + \alpha(i,j)wv(i,j,n) + \beta(i,j)b(i,j,n) \\ Ts(i,j,n+1) \geq Tf(i,j,n) - U(1-wv(i,j,n)) \\ Ts(i,j,n) \geq Tf(i',j,n) - U(1-wv(i',j,n)) \\ Ts(i,j,n) \geq Tf(i',j',n) - U(1-wv(i',j',n)) \\ Ts(i,j,n) \leq H, \; Tf(i,j,n) \leq H \end{array}\right)$$

Duration Constraints

M.G.Ierapetritou and C.A.Floudas. *Effective continuous-time formulation for short-term scheduling. 1. Multipurpose batch processes.* 1998

Increased Complexity: Parameter Fluctuations



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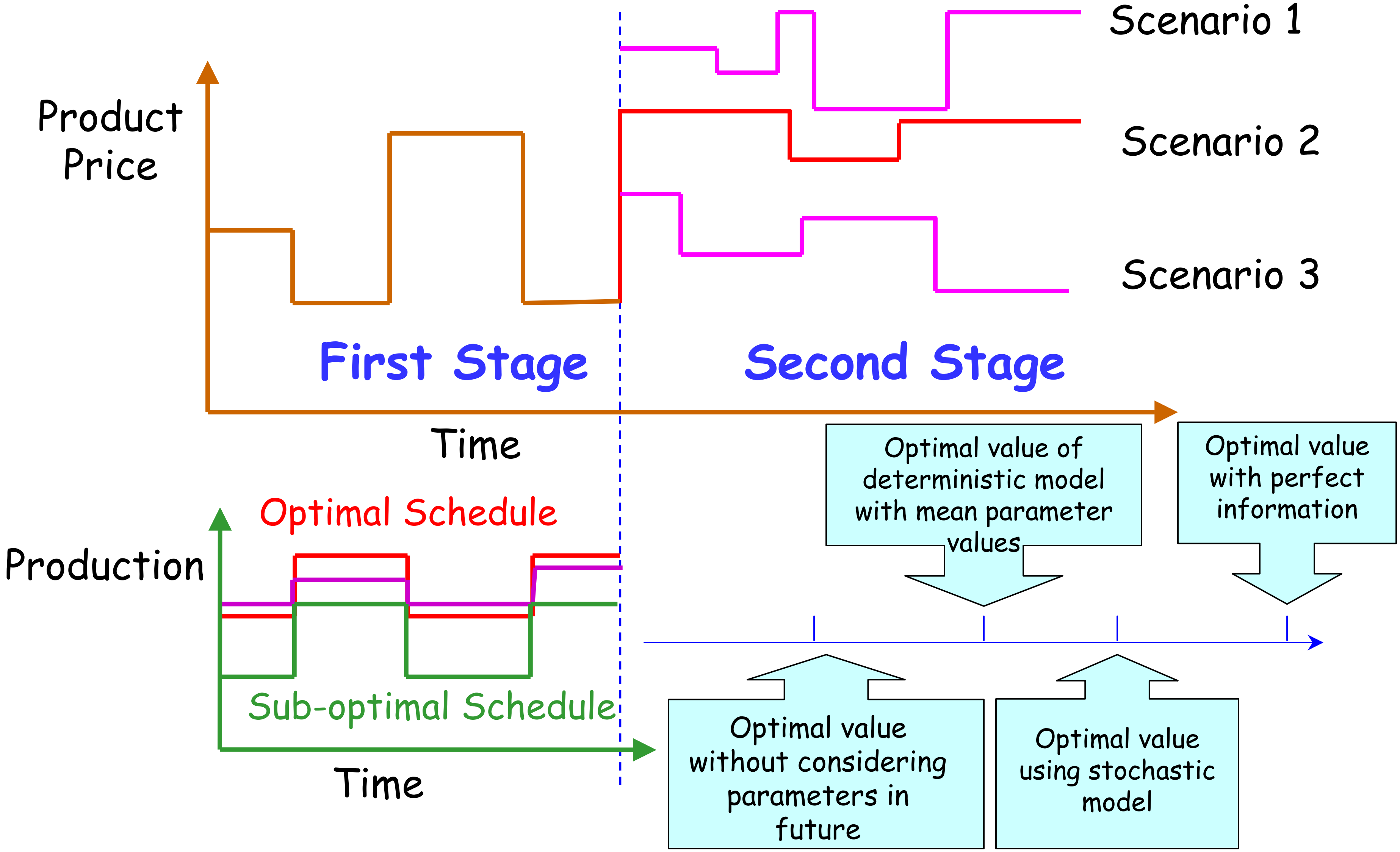
Two-stage Stochastic Approach



Industrial Problem

- **Industry**
  - An air separation company producing large quantities of oxygen, nitrogen and argon
  - Intensive energy consuming process subject to high electricity cost
  - Three operation modes corresponding to different energy consumption levels: regular mode, assisted mode and shutdown mode
- **Objective**
  - Determine the production schedule that minimizes the energy cost while satisfying the demands and other operation consideration
- **Uncertain parameters**
  - **Future energy price**

Solution Approach

- In the first stage, 3-day energy price is assumed deterministic
- Forecasting techniques are utilized to generate scenarios of energy price for the next 5 days
- In the second stage, 5-day stochastic model is considered involving all the scenarios
- Energy cost in both stages are combined in the objective function. The solution provides the schedule of the first 3 days

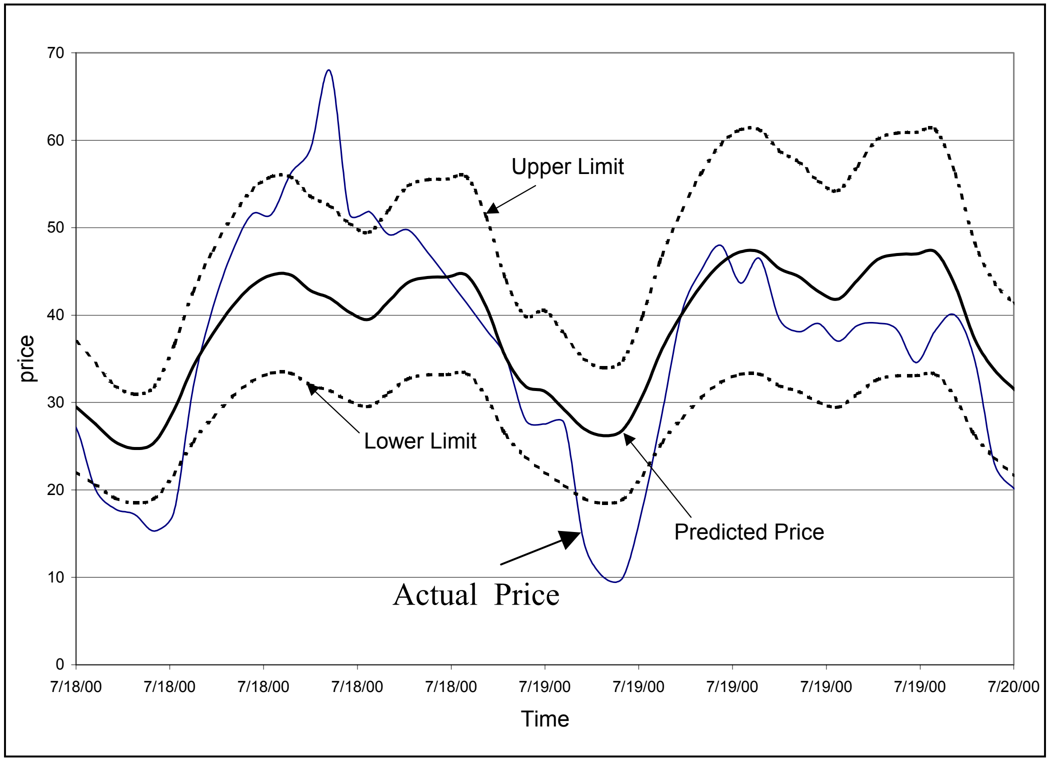
Forecasting Techniques

Energy price series--- no obvious seasonal pattern, unable to be approximated by linear and quadratic terms

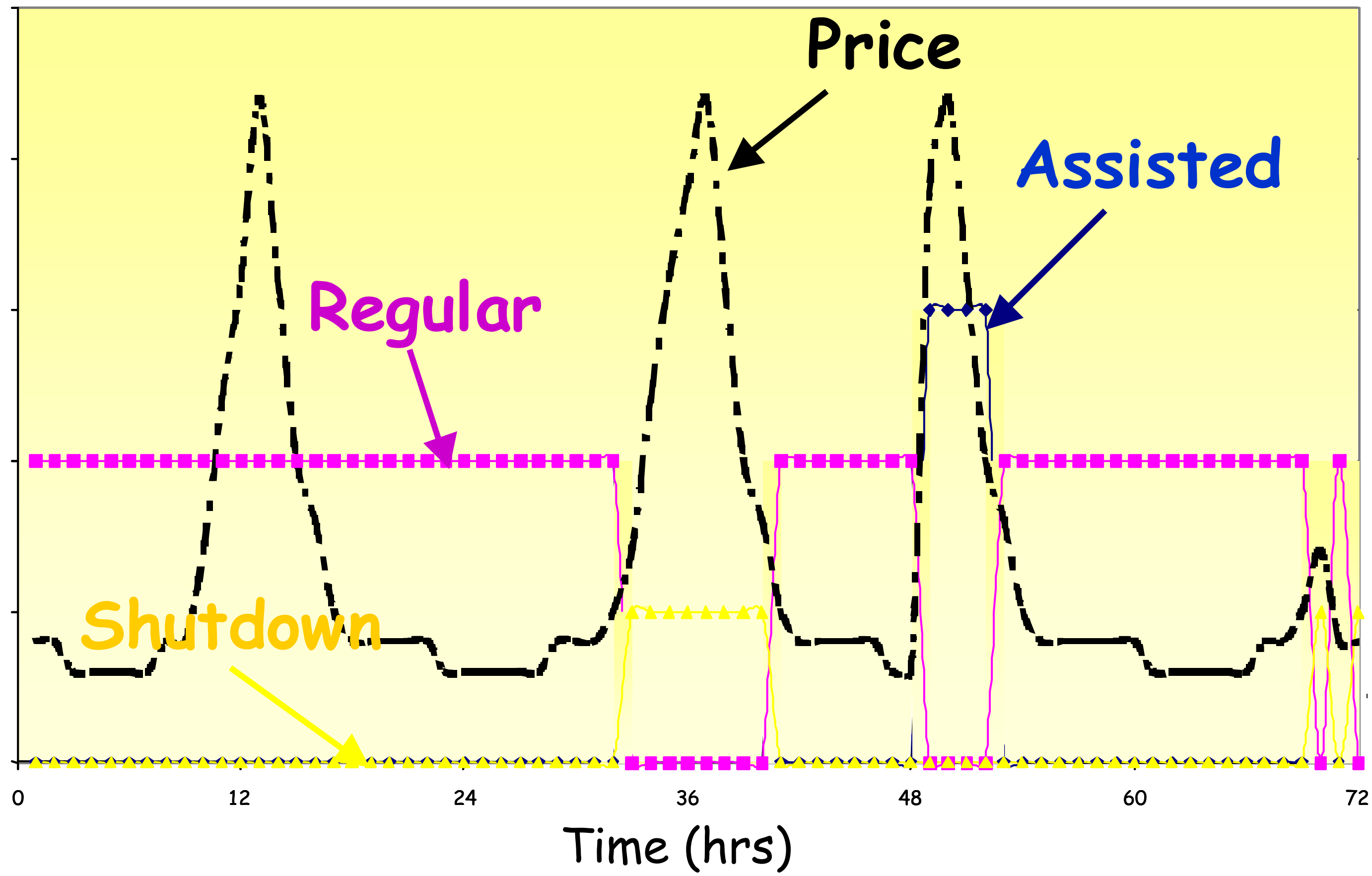
Daily value prediction ------ ARIMA model

Hourly value prediction ----- Hourly Pattern

Two-day price predicted with 95% confidence interval by ARIMA(2,1,1) model



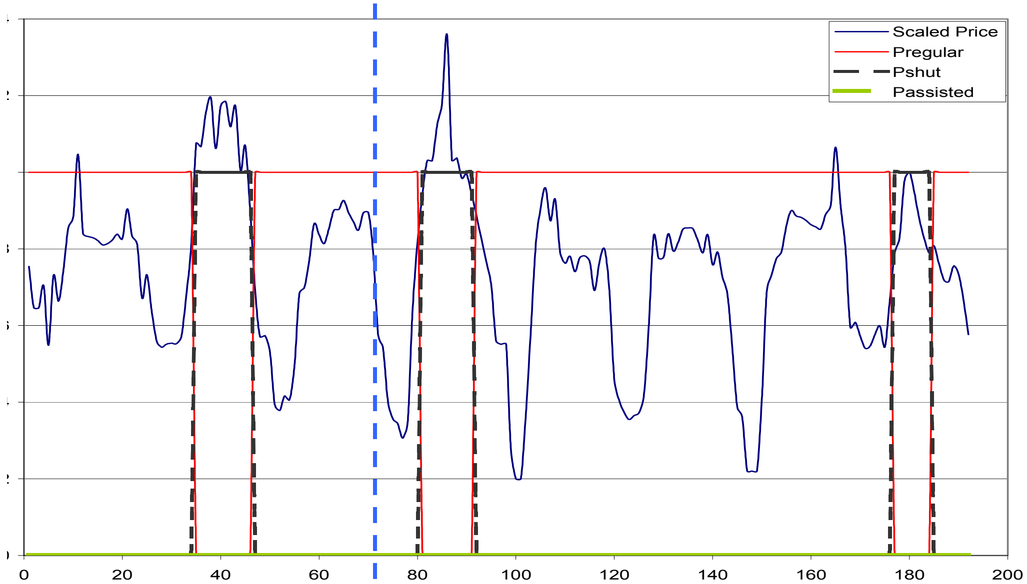
Case Study: Energy Intensive Industrial Plant



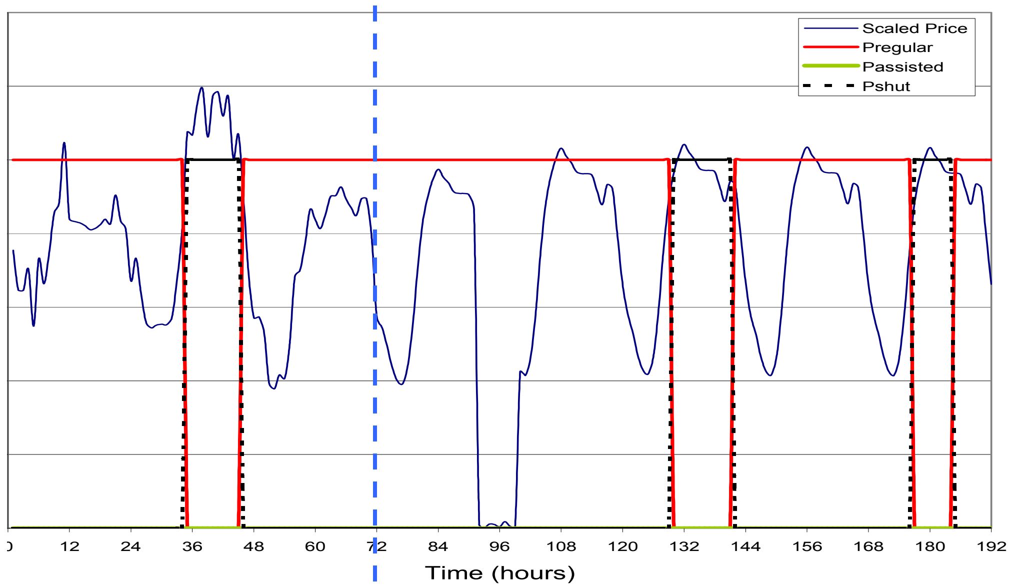
Minimize power cost by switching between different operation modes while satisfying customer requirements

Two-stage Approach considering forecasting prices

Results Comparison



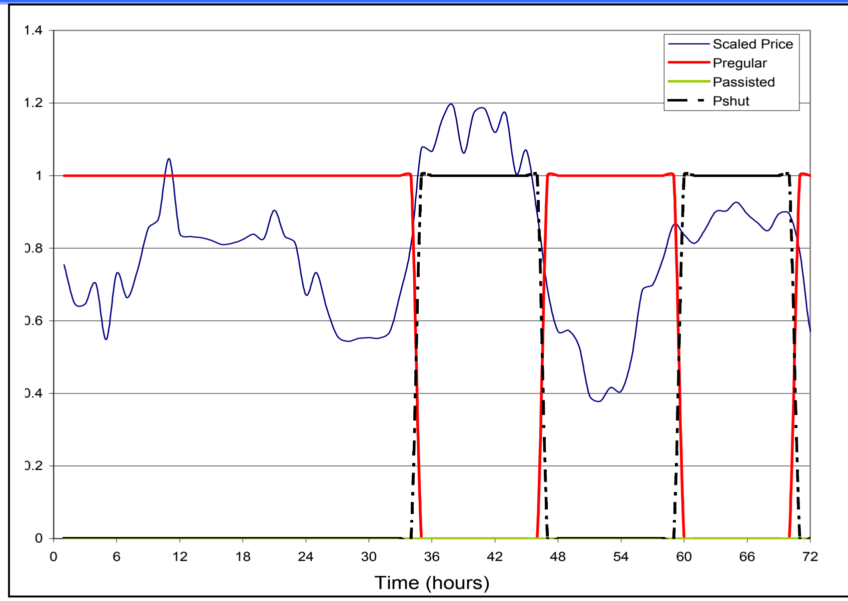
With limited ability to reduce forecasting error, how effective is the proposed two-stage stochastic approach?



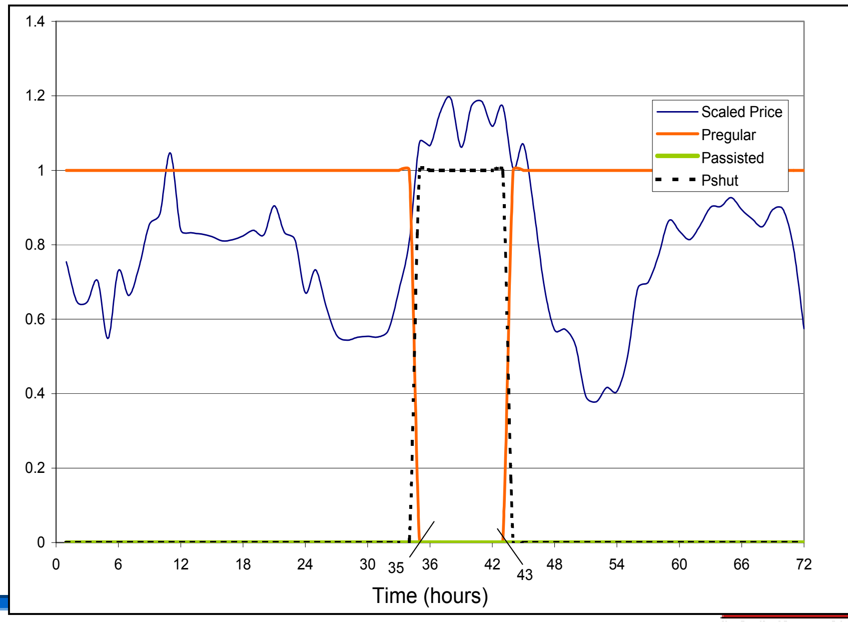
The first 3 days schedule determined using the proposed approach is the same as the optimal schedule using the actual energy prices

Results: Comparison

How is the result compared to the schedule determined without considering future price variation?



The schedule achieved without considering the second stage is more sensitive to the variation of the price



More conservative schedule is determined with the two-stage approach

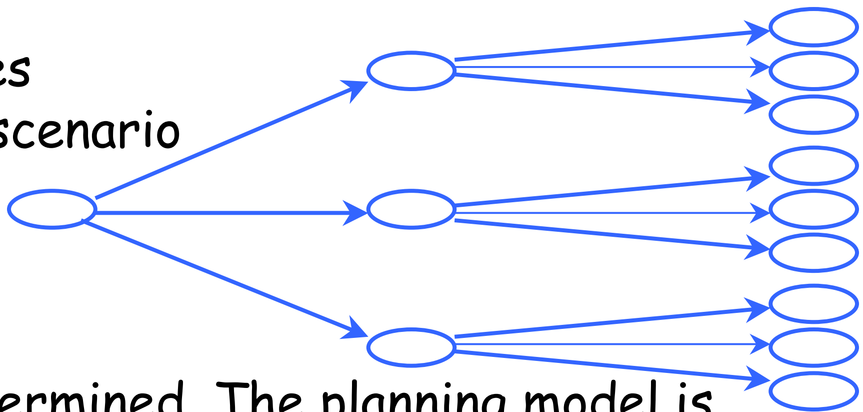
Planning Level

Objective: Determine the aggregated demands for each period

- considering increasing uncertainties along future time periods
- based on material balance

Multi-stage Programming

- Scenarios representing possible values
- One schedule corresponding to each scenario



Rolling Horizon

The schedule of current period is determined. The planning model is moving to the next time point with new data and production results from the scheduling problem.

Sequence Factor

- Account for the impact of recipe complexity
- Simplify the model and reduce the size of the problem

$$\sum_{task} procs\_time \leq \sigma \times H \qquad \textit{for each unit}$$

Scheduling Level

Objective: **Determine the production schedule that**

- **satisfies the orders for the current period**
- **produces the internal demands for the future time**

Continuous-time Formulation

Constraints: *Production* $\geq$ *order in current period*

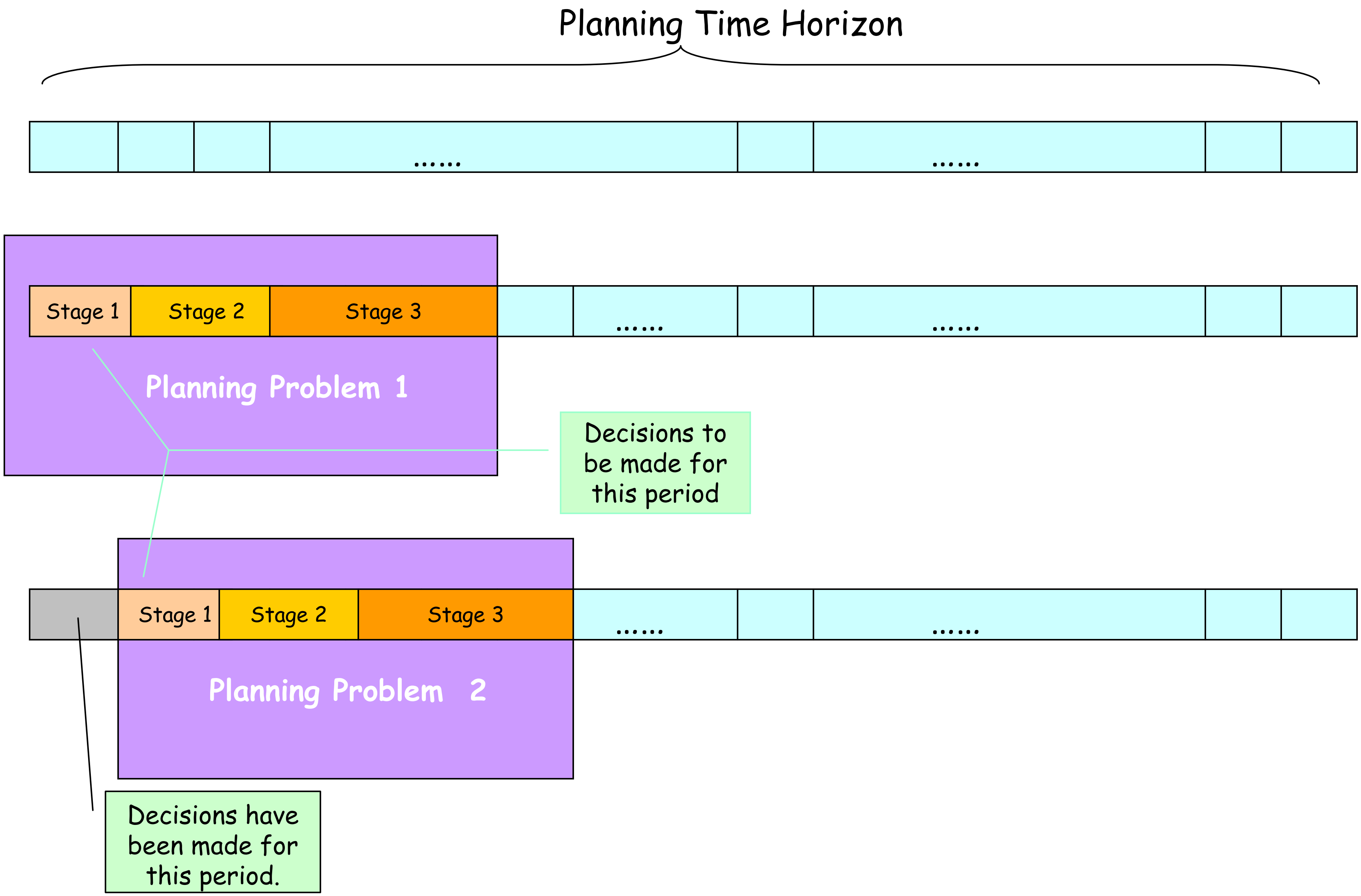
Production $\geq$ *demand from planning results - Slack*

Objective function: *Min priority* $\times$ *Slack*

Infeasibility

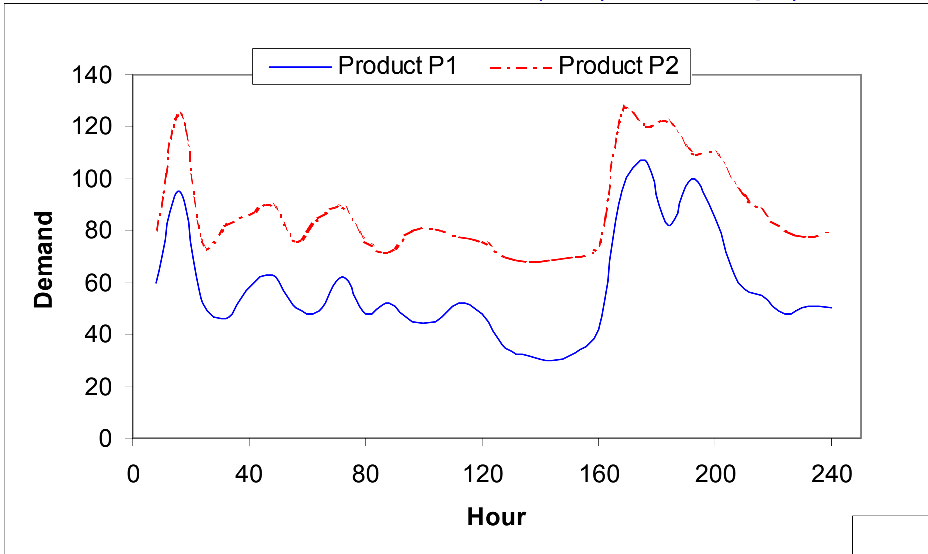
- Allow backorders
- Resolve the planning model and produce the backorder in the nearest period
- Adjust the sequence factor and forecasting scenarios such that they represent better the actual situation

Rolling Horizon Strategy



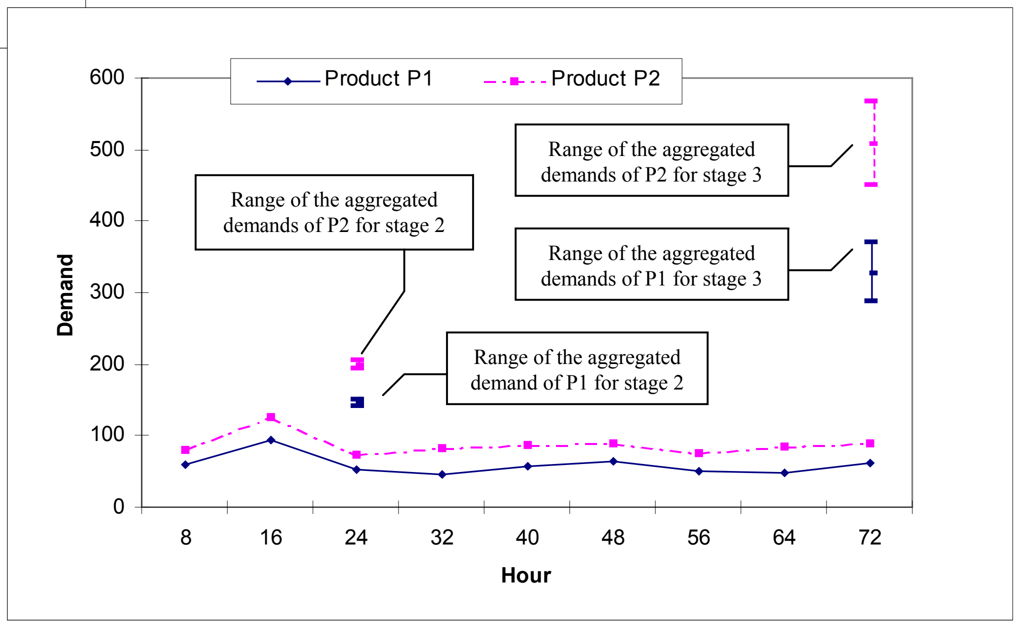
Case Study

10 days planning period: 8 hours schedule

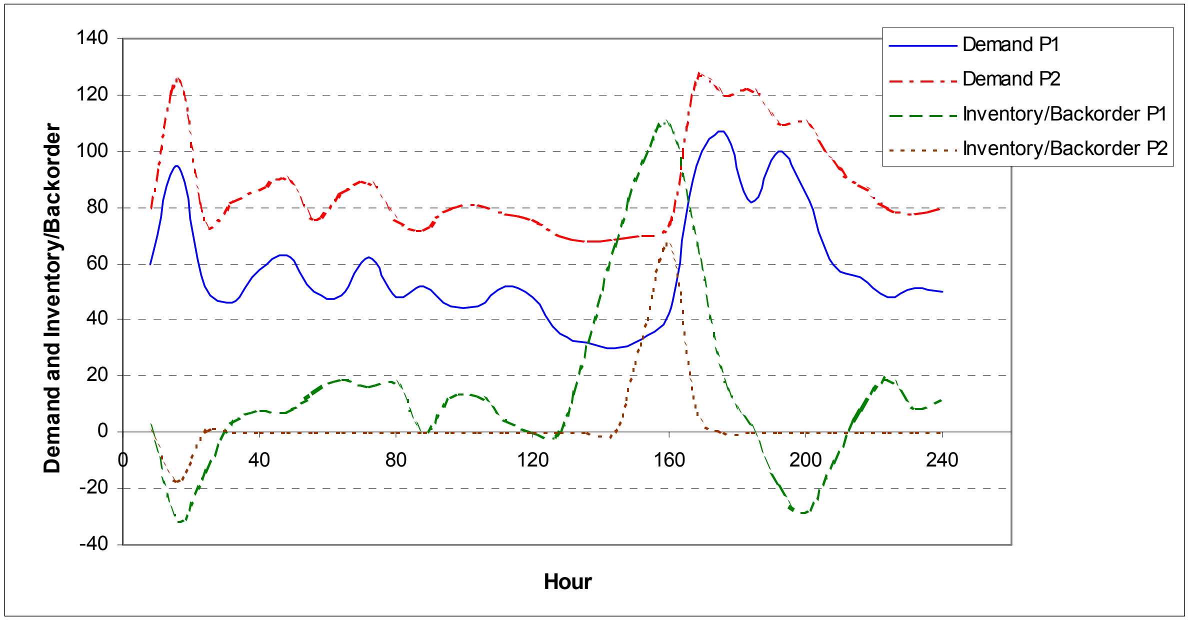


Market Orders (at the end of each period)

Aggregated market orders for the first planning problem

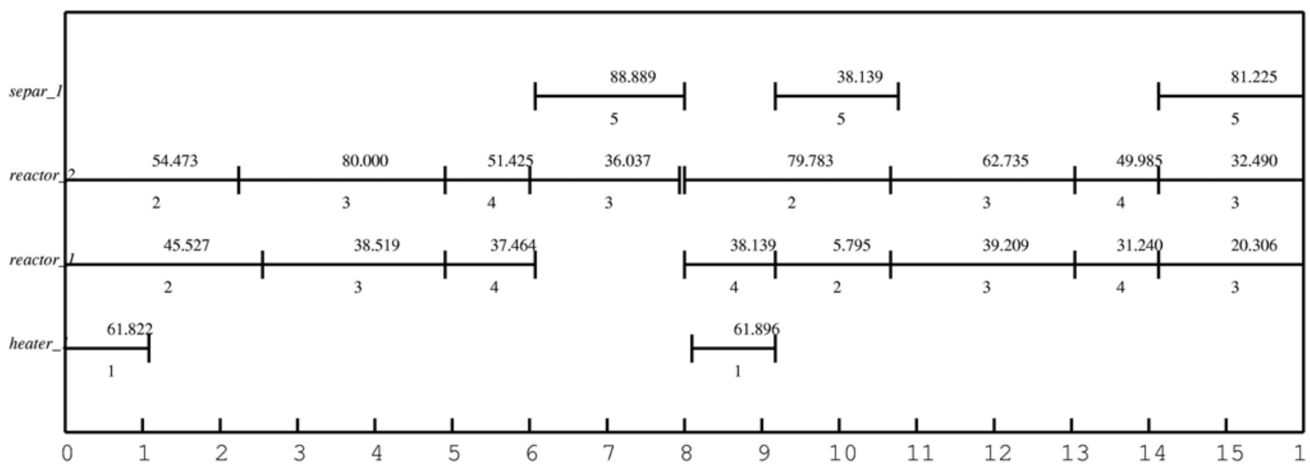


Results



The inventory is compensating against the upcoming demand peaks

The Gantt-chart for the first sixteen hours



Results

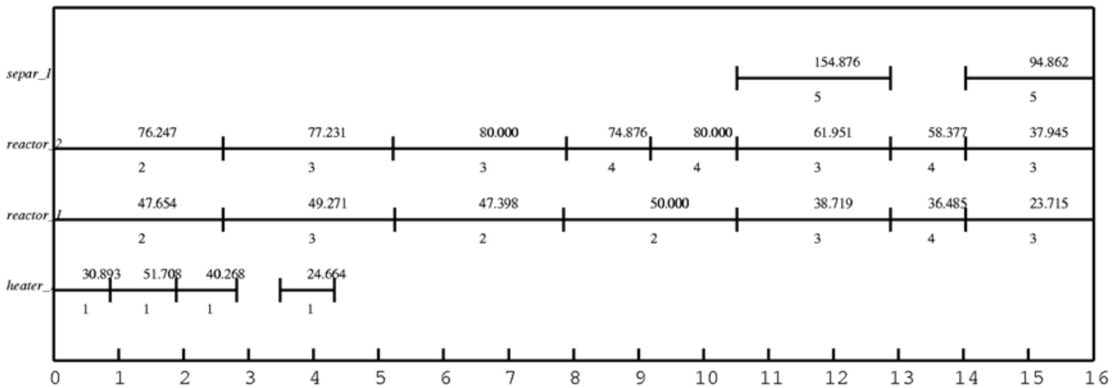
The following three approaches are implemented based on the rolling horizon strategy

- Solve the scheduling problem for each period directly
- Solve the scheduling problem for each two periods directly
- Use proposed hierarchical approach and consider current stage, near stage, future stage with 1, 2 and 6 time periods respectively

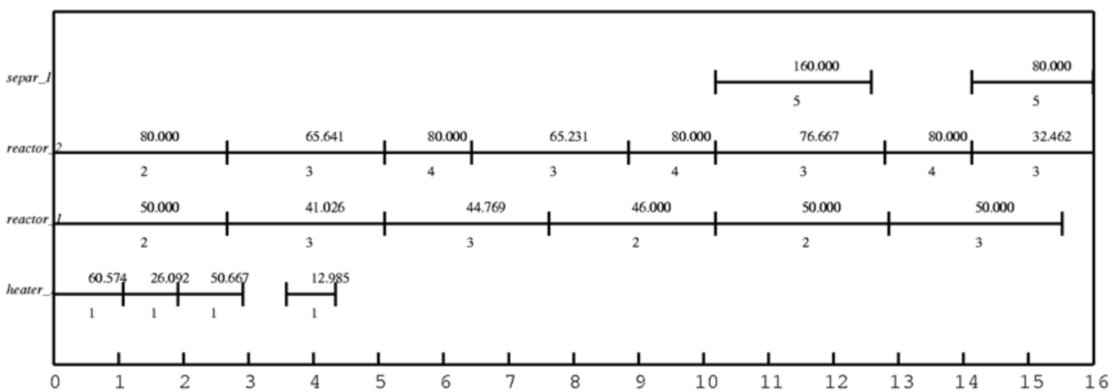
	Oneperiod Scheduling Approach	**Twoperiod Scheduling Approach**	**Proposed Approach**
Time periods with backorders	12	9	5
CPU (sec.)	837	111,104*	1,017
Objective value	112,011.9	46,002.8	28,804.1

Uncertainty in Short-Term Scheduling

Price of P1 is an uncertain parameter. Considering time horizon of 16 hours, $1 increase results in the following different production schedules.



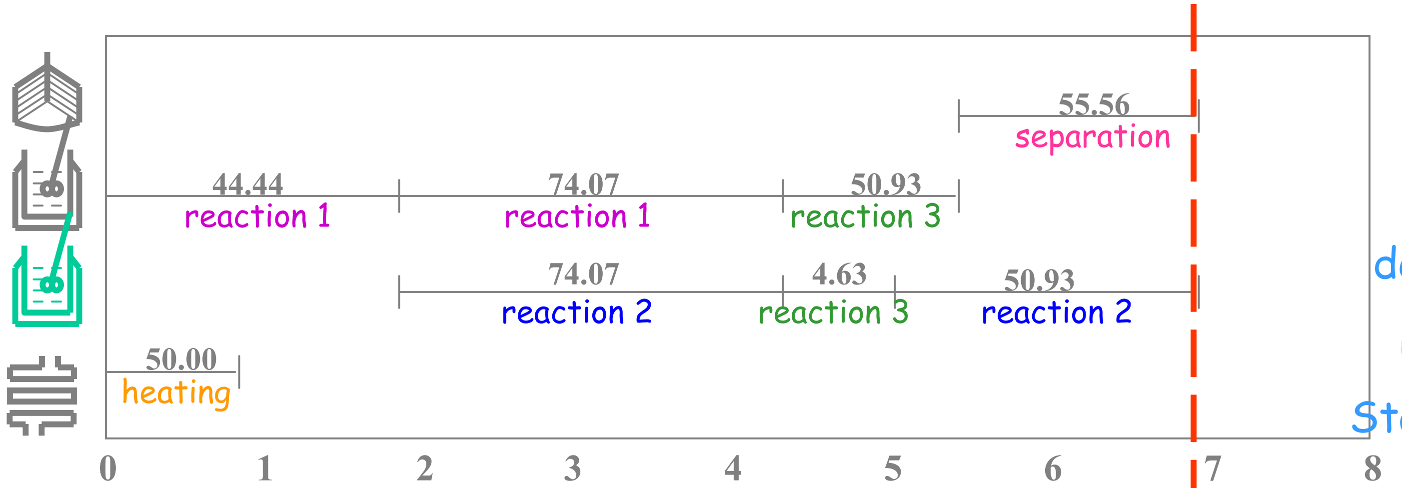
	P1	P2
Price	$10	$10
Production	147.533	224.764



	P1	P2
Price	$11	$10
Production	150.318	216.000

Uncertainty impacts the optimal schedule

Uncertainty in Short-Term Scheduling

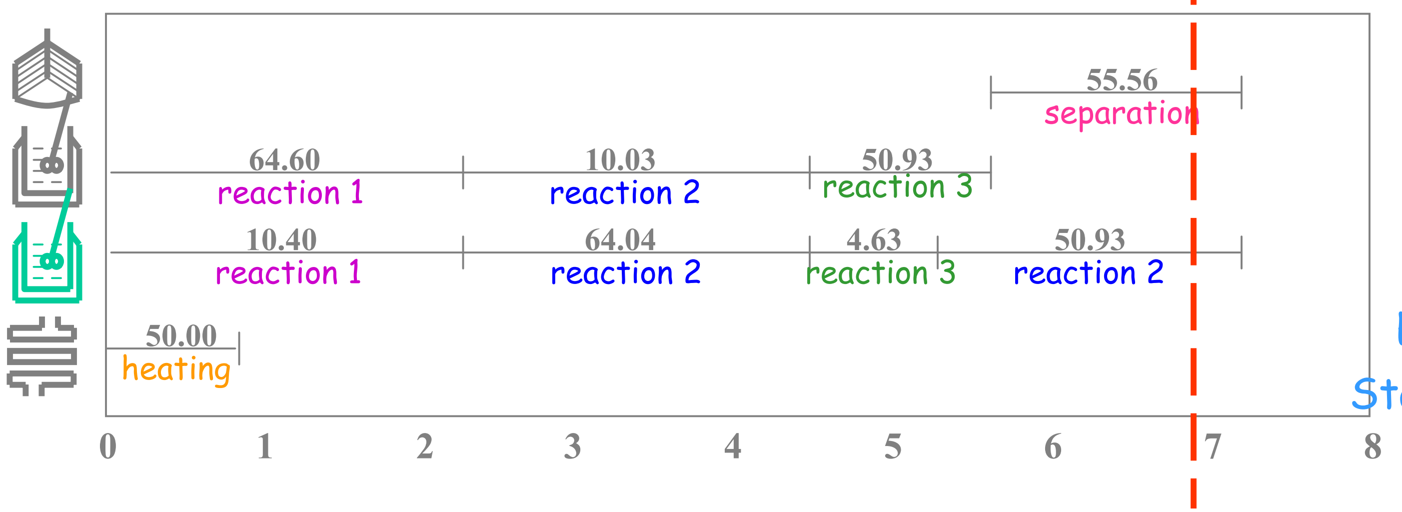


Deterministic Schedule

demand (product 2) = 50

E(makespan) = 8.15hr

Standard Deviation = 2.63



Robust Schedule

demand (product 2) = 50*(1 ± 60%)

E(makespan) = 7.24hr

Standard Deviation = 0.29

Uncertainty in Scheduling

Disruptive Events

Rush Order Arrivals
Order Cancellations
Machine Breakdowns

Not much information is available

REACTIVE SCHEDULING

Parameter Uncertainty

Processing times
Demand of products
Prices

Information is available

PREVENTIVE SCHEDULING

Literature Review: Representative Publications

➢ Reactive Scheduling

Handles uncertainty by adjusting a schedule upon realization of the uncertain parameters or occurrence of unexpected events

❖ S.J.Honkomp, L.Mockus, and G.V.Reklaitis. *A framework for schedule evaluation with processing uncertainty*. Comput. Chem. Eng. 1999, 23, 595

❖ J.P.Vin and M.G.Ierapetritou. *A new approach for efficient rescheduling of multiproduct batch plants*. Ind. Eng. Chem. Res., 2000, 39, 4228

➢ Stochastic Programming

Uncertainty is modeled through discrete or continuous probability functions

❖ J.R.Birge and M.A.H.Dempster. *Stochastic programming approaches to stochastic scheduling*. J. Global. Optim. 1996, 9, 417

❖ J.Balasubramanian and I.E.Grossmann. *A novel branch and bound algorithm for scheduling flowshop plants with uncertain processing times*. Comput. Chem. Eng. 2002, 26, 41

Literature Review: Representative Publications

➢ Fuzzy Programming

Considers random parameters as fuzzy numbers and the constraints are treated as fuzzy sets

- H.Ishibuchi, N.Yamamoto, T.Murata and Tanaka H. *Genetic algorithms and neighborhood search algorithms for fuzzy flowshop scheduling problems* . Fuzzy Sets Syst. 1994, 67, 81
- J.Balasubramanian and I.E.Grossmann. *Scheduling optimization under uncertainty- an alternative approach*. Comput. Chem. Eng. 2003, 27, 469

➢ Robust Optimization

Produces "robust" solutions that are immune against uncertainties

- X.Lin, S.L.Janak, and C.A.Floudas. *A new robust optimization approach for scheduling under uncertainty – I. bounded uncertainty*. Comput. Chem. Eng. 2004, 28, 2109

➢ MILP Sensitivity Analysis

Utilizes MILP sensitivity analysis methods to investigate the effects of uncertain parameters and provide a set of alternative schedules

- Z.Jia and M.G.Ierapetritou. *Short-term Scheduling under Uncertainty Using MILP Sensitivity Analysis.* Ind. Eng. Chem. Res. 2004, 43, 3782

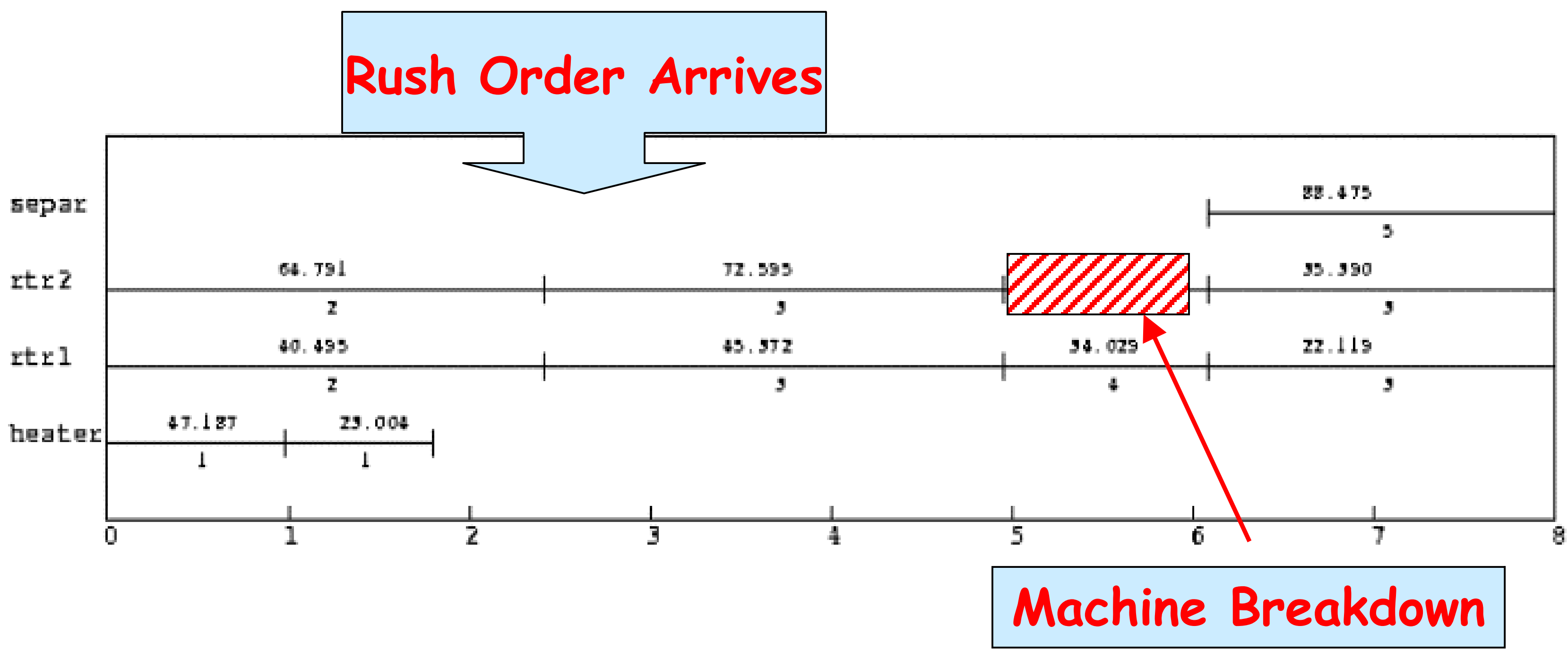
Reactive Scheduling

Common Disruptions

- Rush Order arrivals
- Order Cancellations
- Machine Breakdowns

Key Features

- Handles the disturbance at the time it occurs
- Meet new and existing requirements
- Maintain smooth plant operation



Reactive Scheduling Approach

Vin and Ierapetritou Ind. Eng. Chem. Res. 2000

Until the time of disturbance – original schedule is followed
- fixing binary and continuous variables

DATA

Shift starting times to account for breakdown

DETERMINISTIC MODEL

Modify demand constraint

CONSTRAINTS

CONSTRAINTS

Take care of any infeasibilities: change the objective function
Maintain smooth plant operation

Machine Breakdown

Fix binary variables to comply with original schedule:
- for unit that breaks : fix all tasks that have finished before T_{break}
- for other units: fix all tasks that have started before T_{break}

Modify time constraints to shift starting times
for all event points on which tasks have not yet started

$$T^{sr1}(i,j,n_b) \geq T_{break} + T_{maint}$$

Minimize the differences between reschedule and original schedule:

$$\text{Maximize } \sum \sum \text{price}(s)d(s,n) - \text{penalty}\left(\left(\left| wv^{r1}(i,n) - wv.l(i,n) \right| + \left| yv^{r1}(j,n) - yv.l(j,n) \right| \right) \right.$$

Rush Order Arrival

Fix binary variables to comply with original schedule for all those tasks whose starting times is less than T_{rush}

Alter the demand constraint to account for additional order

$$\sum d(s,n) \geq r^{rush}(s)$$

Modify the objective function to :

maximize $\sum price(s)*priority(s)*d^{r1}(s,n)$

$- penalty* \sum priority'(s)*slack(s)$

OR

minimize H

Is the problem infeasible?

Yes

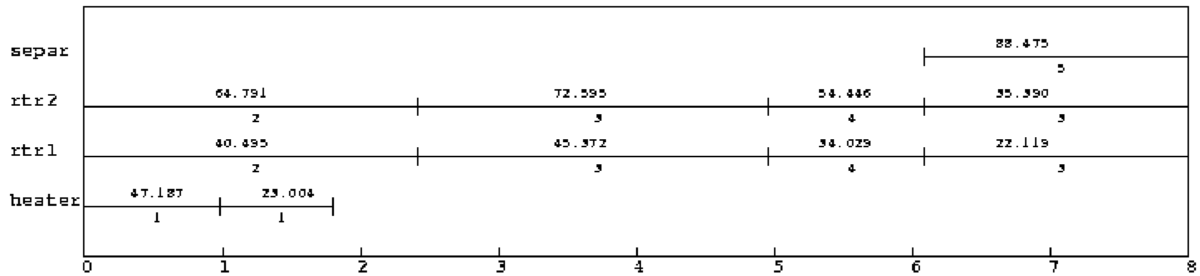
No

Stop

Motivation Example: Machine Breakdown

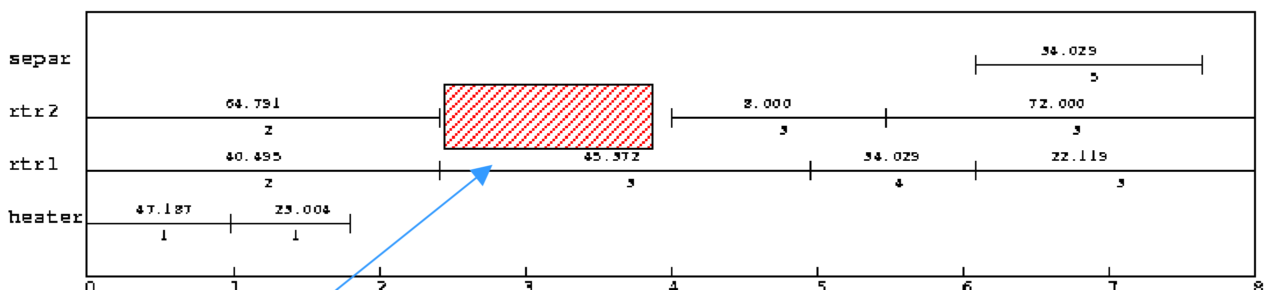
Reactor 2 breaks down at T_{break} = 3 hrs and requires 1 hr maintenance

Deterministic schedule



The profit goes down from 1498 units to 896 units (40%) due to machine breakdown

Reschedule

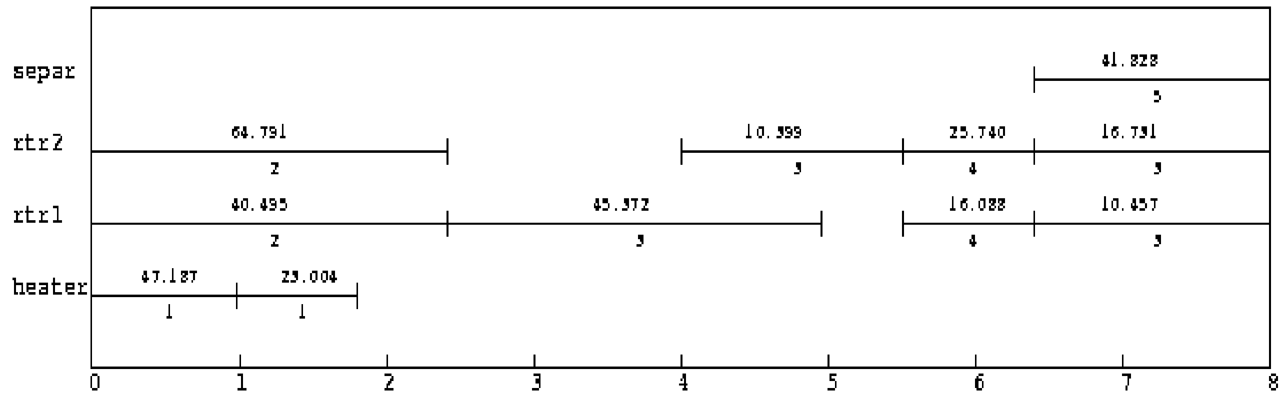


Reactor 2 is inactive

Smooth Plant Operation

Forced using high penalty in the objective function

Profit goes down further to 708 units (52%)



Trade-off between profit and smooth plant operation

Penalty	Profit for Reschedule	Differences in assignments
0	896.23	7
50	896.23	2
100	826.68	1
500	708.29	0
100,000	708.29	0

Key Features of the Approach

- Utilizes all possible information from the deterministic schedule ensuring minimal disruption in plant operation at the time of disturbance

- Although the entire time horizon is considered, fixing the binary variables reduces the size of the problem improving the computational efficiency

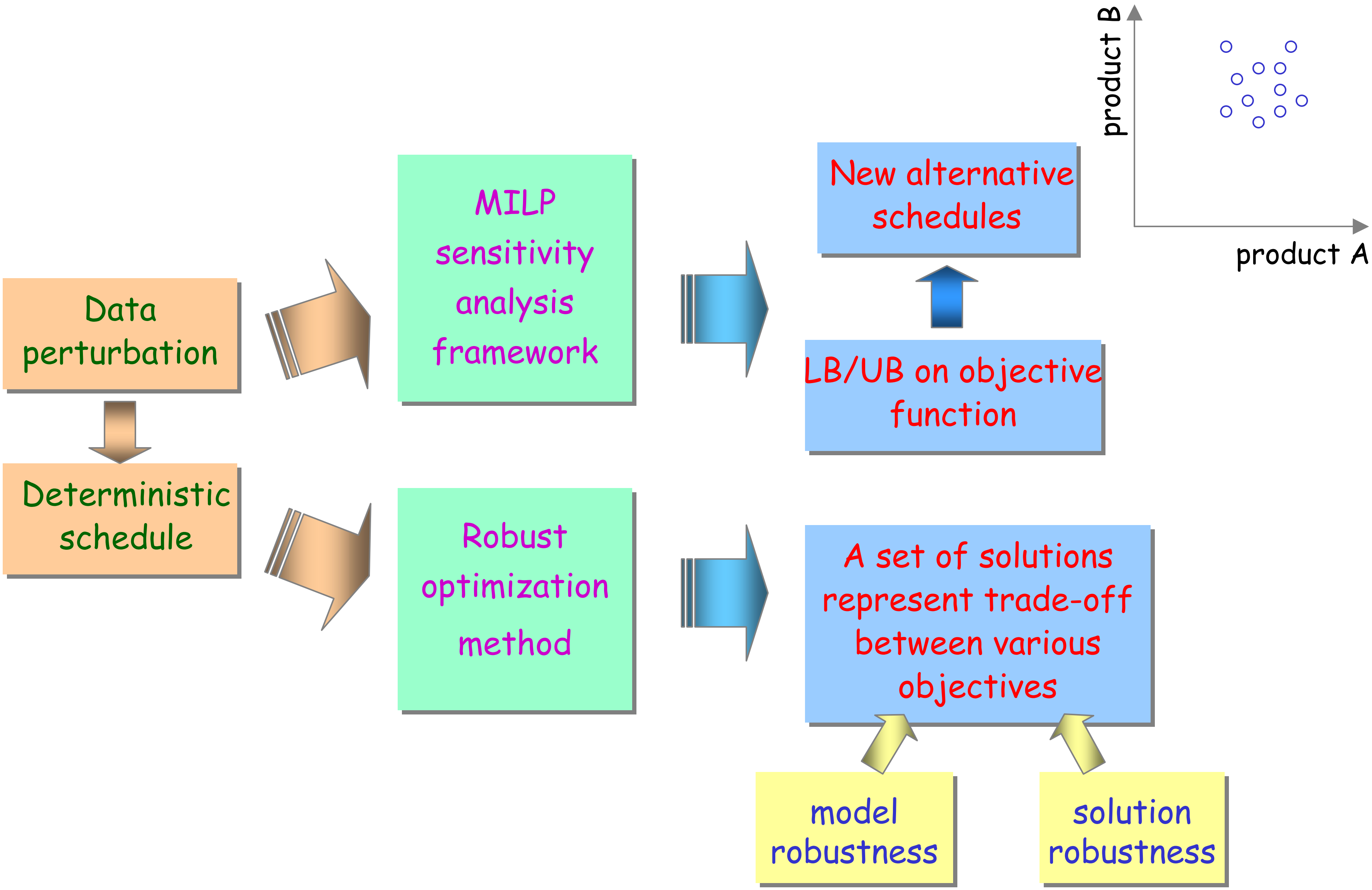
- No heuristics are used in rescheduling; all possible rescheduling alternatives are considered to obtain an optimal solution

- Models the tradeoff between objectives and maintain smooth plant operation – thus allowing the flexibility to balance the two objectives.

- Ability to handle more than one disturbances

Preventive Scheduling

Preventive Scheduling



THE STATE UNIVERSITY OF NEW JERSEY RUTGERS

Preventive Scheduling

➢MILP Sensitivity Analysis

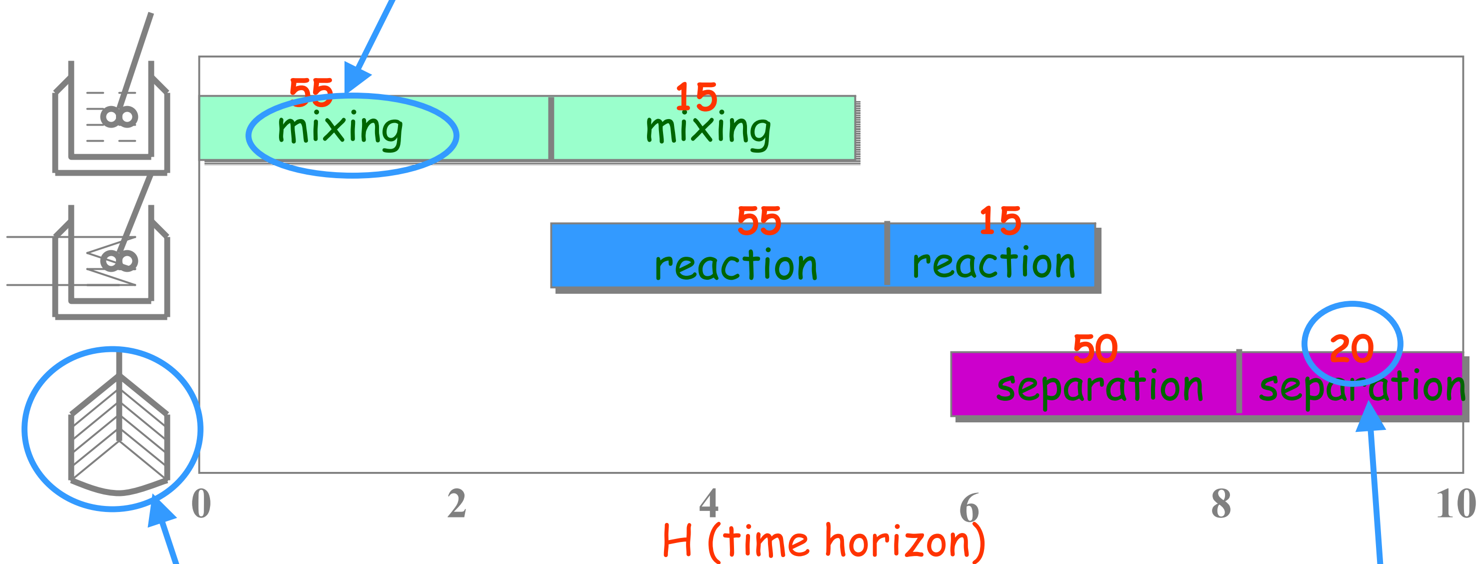
$$\text{minimize } H \quad \text{or} \quad \text{maximize } \sum price(s)d(s,n)$$
$$\text{subject to } \sum wv(i,j,n) \le 1$$
$$st(s,n) = st(s,n-1) - d(s,n) + \sum \rho^{P} \sum b(i,j,n-1) + \sum \rho^{c} \sum b(i,j,n)$$
$$st(s,n) \le stmax(s)$$
$$Vmin(i,j)wv(i,j,n) \le b(i,j,n) \le Vmax(i,j)wv(i,j,n)$$
$$\sum d(s,n) \ge r(s)$$
$$Tf(i,j,n) = Ts(i,j,n) + \alpha(i,j)wv(i,j,n) + \beta(i,j)b(i,j,n)$$
$$Ts(i,j,n+1) \ge Tf(i,j,n) - U(1-wv(i,j,n))$$
$$Ts(i,j,n) \ge Tf(i',j,n) - U(1-wv(i',j,n))$$
$$Ts(i,j,n) \ge Tf(i',j',n) - U(1-wv(i',j',n))$$
$$Ts(i,j,n) \le H, \; Tf(i,j,n) \le H$$

Mixed-integer Linear Programming

➢Robust Optimization

Questions to Address

- What is the effect of processing time at the objective value?



-How the capacity of the units affect the production objective?

-Can the schedule accommodate the demand fluctuation?

Parametric Programming

$$z(\theta) = \min \; c^T x + d^T y$$
$$\text{subject to} \quad Ax + Dy \le b$$
$$x^L \le x \le x^U$$
$$\theta^L \le \theta \le \theta^U$$
$$x \in R^m, \; y \in (0,1)^T$$

$b = b_0 + \theta r \quad b \in [b_0 + \theta^L r, \; b_0 + \theta^U r]$

solved at $b = b_0 + \theta^L r$
optimal solution (x^*, y^*)

Fix integer variables at y^*

LP sensitivity analysis:
$z(\theta) = z_0 + \lambda\theta$
$\theta^L \le \theta^{L\prime} \le \theta \le \theta^{U\prime} \le \theta^U$

$$z(\theta) = \min \; c^T x + d^T y$$
$$\text{subject to} \quad Ax + Dy - \theta r \le b$$
$$c^T x + d^T y - z_0 - \lambda\theta = 0$$
$$\sum_{i \in F^1} y_i - \sum_{i \in F^0} y_i \le |F^1| - 1$$
$$x^L \le x \le x^U$$
$$\theta^{L\prime} \le \theta \le \theta^{U\prime}$$
$$x \in R^m, \; y \in (0,1)^T$$

Integer cut to exclude current optimal solution

break point θ', new
optimal solution $(x^{*\prime}, y^{*\prime})$

A.Pertsinidis et al. Parametric optimization of MILP progarms and a framework for the parametric optimization of MINLPs. 1998

Inference-based MILP Sensitivity Analysis

minimize $z = cx$
subject to $Ax \geq a$
$0 \leq x \leq h$, x_j integer, $j=1,\ldots k$

minimize $z = (c + \Delta c)x$
subject to $(A + \Delta A)x \geq a + \Delta a$
$0 \leq x \leq h$, x_j integer, $j=1,\ldots k$

Aim: Determine under what condition $z \geq z^* - \Delta z$ remains valid

Partial assignment at node p $\quad x_j \in \{\underline{u}_j^P, \ldots, \overline{u}_j^P\} \quad j = 1,\ldots,n$

Bound $z \geq z^* - \Delta z$ holds if there are $s_1^P, \ldots, s_n^P$ that satisfy:

- for the perturbations ΔA and Δa

$$\lambda_i^P \sum A_{ij}\underline{u}_j^P + \sum s_j(\overline{u}_j - \underline{u}_j) - \lambda_i \Delta a_i \leq r^P$$

$$s_j^P \geq \lambda_i^P \Delta A_{ij},\ s_j^P \geq -q_j^P,\ j = 1,\ldots,n$$

$$r^P = -\sum q_j^P u_j^P + \lambda^P a - z^P + \Delta z^P$$

- for the perturbations Δc

$$\sum \Delta c_j \underline{u}_j^P - s_j^P(\overline{u}_j^P - \underline{u}_j^P) \geq -r^P$$

$$s_j^P \geq -\Delta c_j,\ s_j^P \geq -q_j^P,\ j = 1,\ldots,n$$

$$q_j^P = \lambda_i^P A_{ij} - \lambda_i^P c_j$$

*M.W.Dawande and J.N.Hooker, 2000

Proposed Uncertainty Analysis Approach

Solve the deterministic scheduling problem using B&B tree

Extract information from the leaf nodes

- Range of parameter change for certain objective change
- Important parameters
- Plant robustness

Move the bounds of the uncertainty parameter range

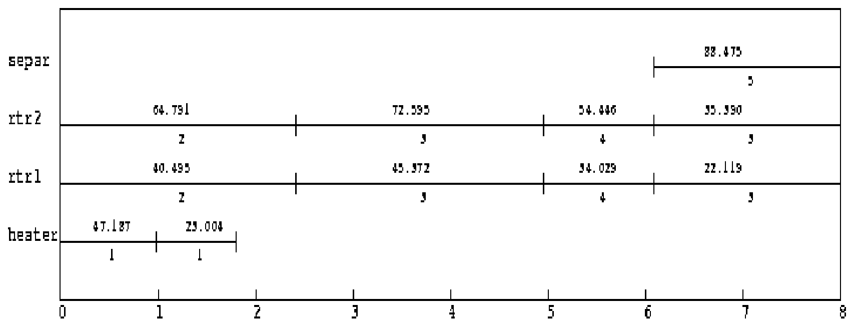
Identify the feasible schedules by examining the B&B tree

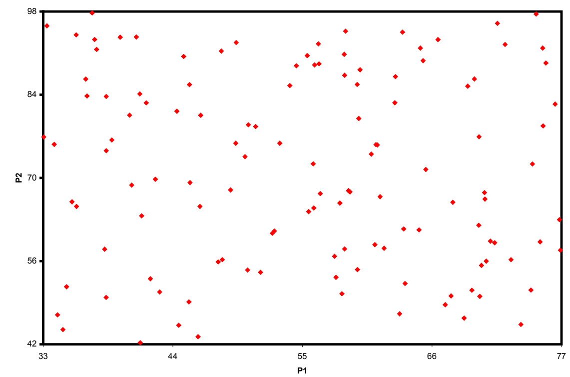
Evaluate the alternative schedules

- Robustness
- Nominal performance
- Average performance

Robustness Estimation

Makespan minimization is considered as the objective





Obtain sequence of tasks from original schedule

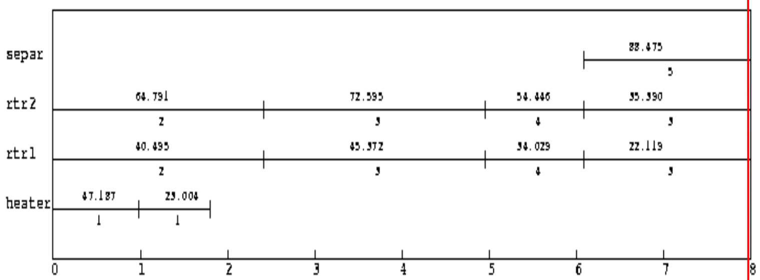
Generate random demands in expected range

Makespan to meet a particular demand is found using the sequence of tasks derived from original schedule

Binary variables corresponding to allocation of tasks are fixed

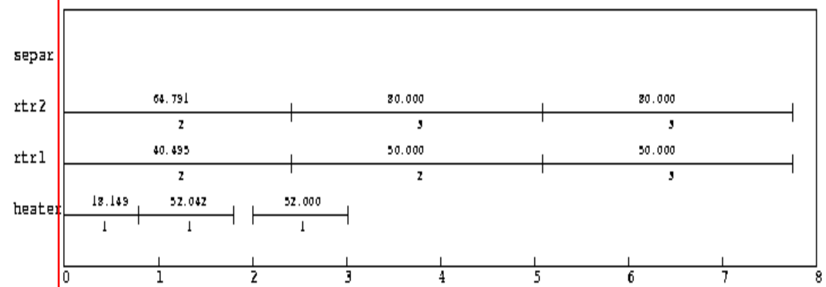
Batch sizes and Starting and Finishing times of tasks are allowed to vary

Robustness under Infeasibility



Inventory of raw materials intermediates etc.

ROLLOVER



H_{max}

Meets maximum possible demand

H_{inf}

Meets unsatisfied demand

Total makespan $H_{corr} = H_{max} + H_{inf}$

Corrected Standard Deviation:

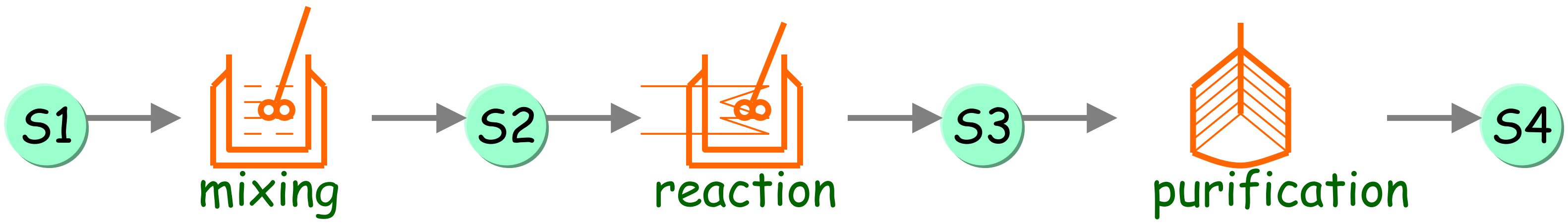
$$SD_{corr} = \sqrt{\sum_{p=1}^{p_{tot}} \frac{(H_{act} - H_{\det})^2}{(p_{tot} - 1)}}$$

$H_{act} = H_p$ if scenario is feasible

$= H_{corr}$ if the scenario is infeasible

J.P.Vin and M.G.Ierapetritou. *Robust short-term scheduling of multiproduct batch plants under demand uncertainty*. 2001

Case Study 1

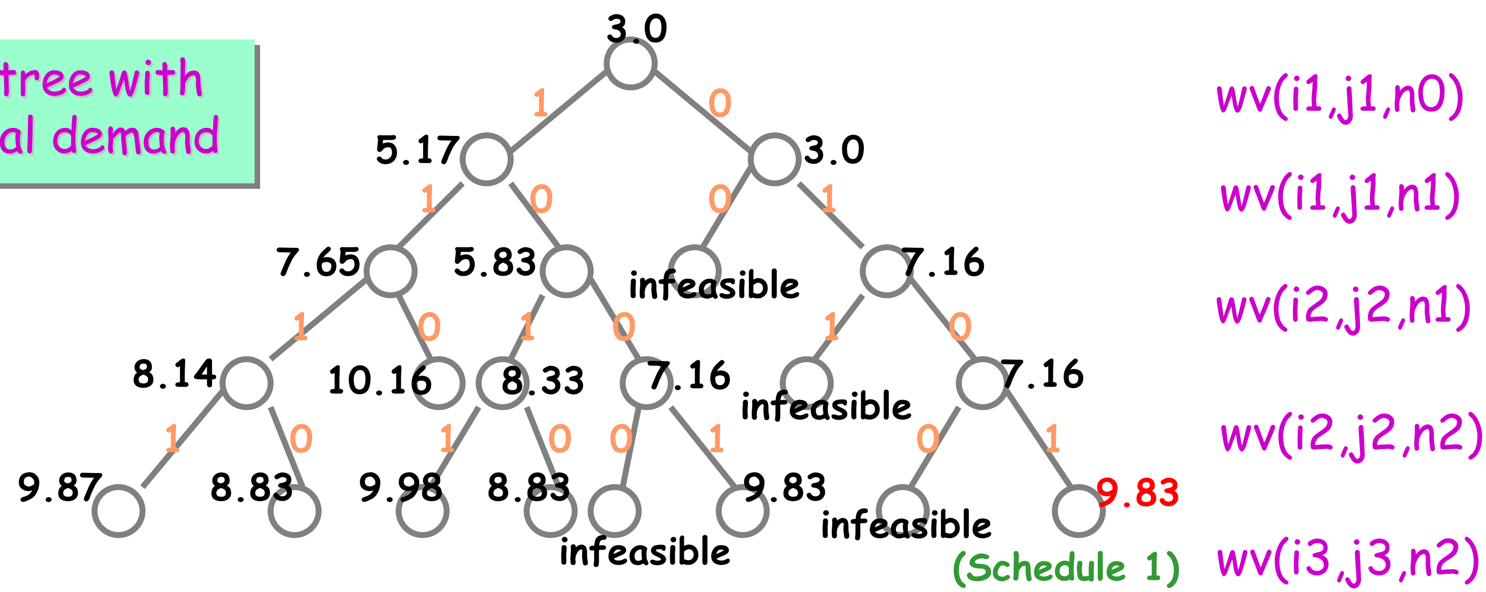


Effect of demand d~[20, 100]

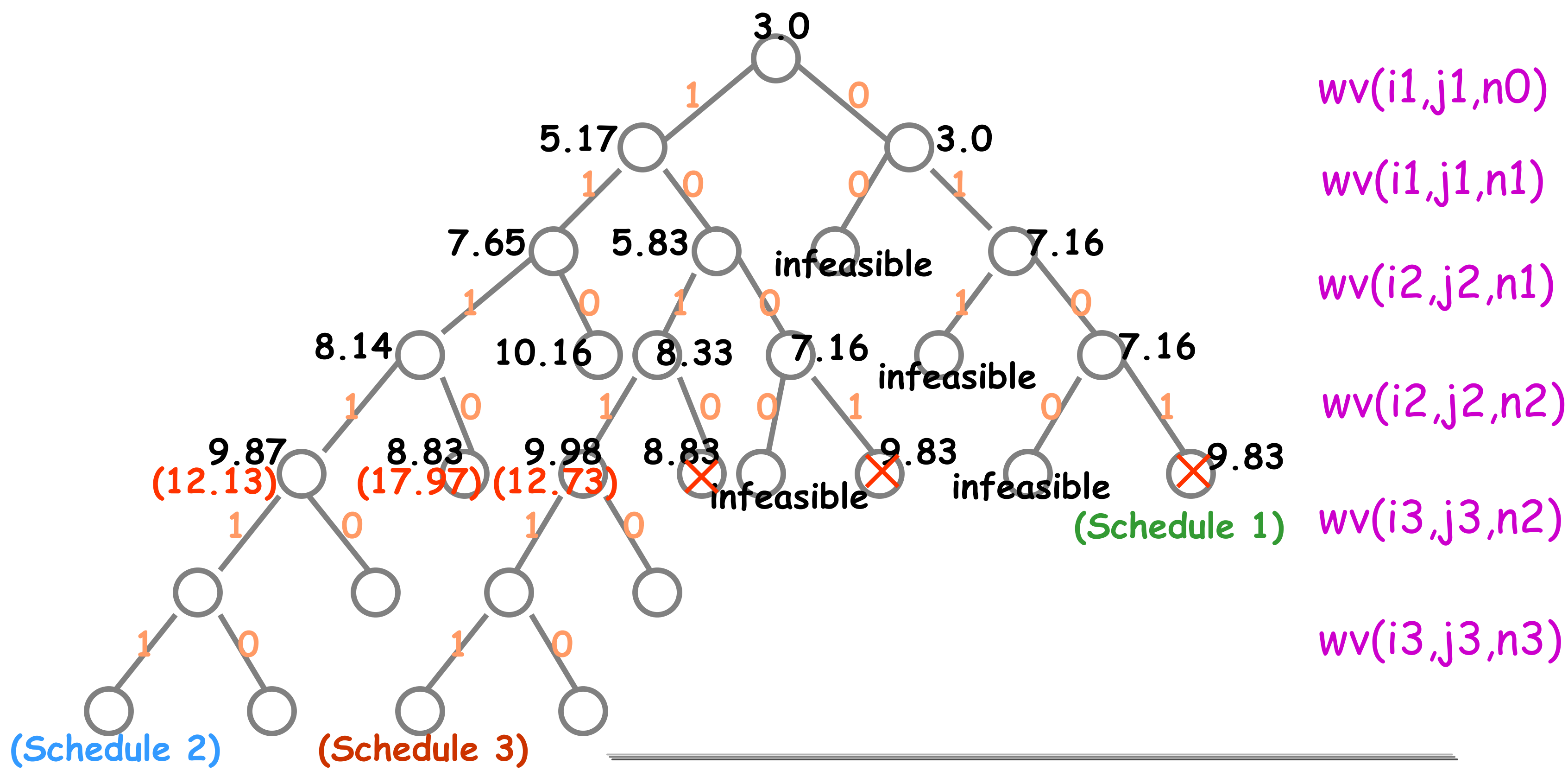
$d_{nom} = 50 \quad H_{nom} = 9.83h \quad -0.097\ \Delta d \leq \Delta H$

$d' = 80 \quad H' \leq H_{nom} + 0.097\Delta d = 12.73h$

B&B tree with nominal demand



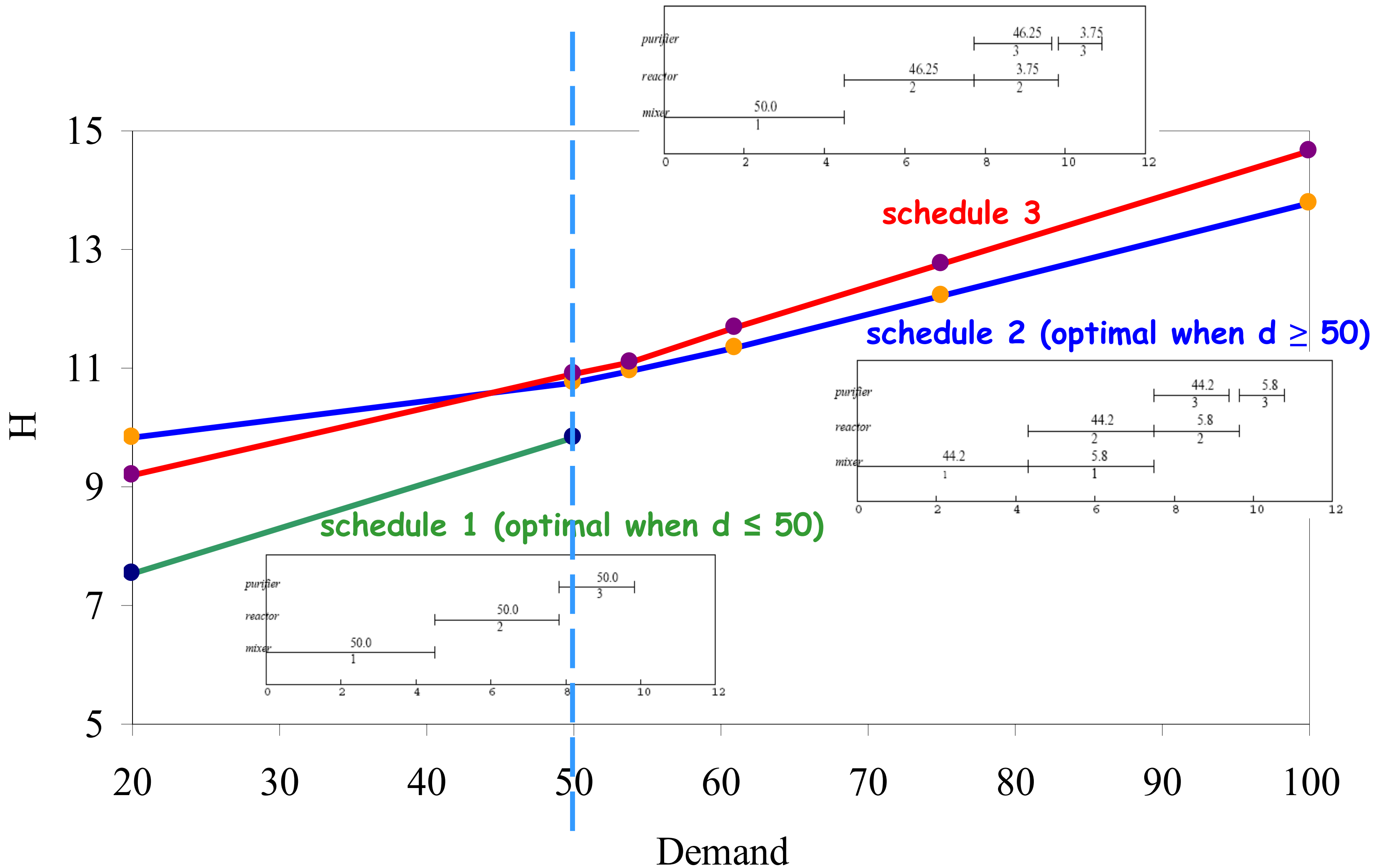
Case Study 1



Schedule Evaluation

	schedule 1	schedule 2	schedule 3
H_{nom}(h)	9.83	10.77	10.91
H_{avg}(h)	14.20	11.56	11.79
SD_{corr}	5.52	1.61	2.17

Case Study 1



purifier
reactor
mixer
46.25
3
3.75
3
46.25
2
3.75
2
50.0
1
0
2
4
6
8
10
12
15
13
11
9
7
5
H
schedule 3
schedule 2 (optimal when d ≥ 50)
44.2
3
5.8
3
44.2
2
5.8
2
44.2
1
5.8
1
schedule 1 (optimal when d ≤ 50)
50.0
3
50.0
2
50.0
1
20
30
40
50
60
70
80
90
100
Demand

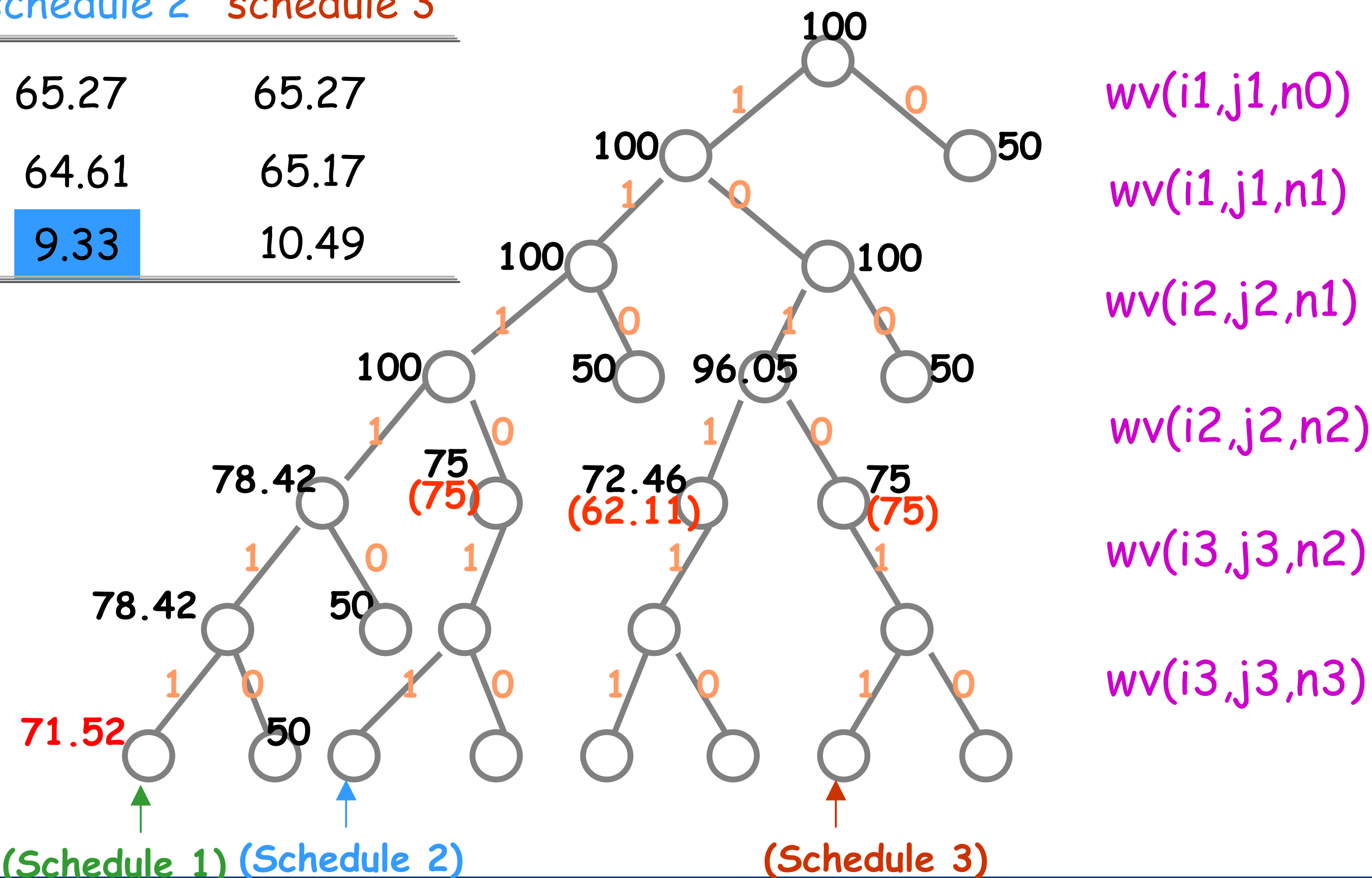
Case Study 1

Effect of processing time $T(i1,j1) \sim [2.0, 4.0]$

$T_{nom} = 3.0$ $\quad$ $profit_{nom} = 71.52$

$T' = 4.0$ $\quad$ $profit' \geq profit_{nom} + 24.48\Delta T = 47.04$

	schedule 1	schedule 2	schedule 3
$profit_{nom}$	71.52	65.27	65.27
$profit_{avg}$	66.98	64.61	65.17
SD_{corr}	26.9	9.33	10.49



Preventive Scheduling

- MILP Sensitivity Analysis
- **Robust Optimization**

Objective = { Expected Makespan/Profit; Model Robustness; Solution Robustness }

Robust Optimization

$$\text{minimize} \quad \begin{pmatrix} \sum_k P^k H^k \\ \sum_k P^k \sum_s \textbf{slack}^k(s) \\ \sum_k P^k \Delta^k \end{pmatrix}$$

Average Makespan

Model Robustness

Solution Robustness

subject to $\sum_{(i,j)} wv(i,j,n) \leq 1$

$$st^k(s,n) = st^k(s,n-1) - d^k(s,n) + \sum \rho^P(s,i) \sum b^k(i,j,n-1) + \sum \rho^c \sum b^k(i,j,n)$$

$$st^k(s,n) \leq stmax(s)$$

$$Vmin(i,j)wv(i,j,n) \leq b^k(i,j,n) \leq Vmax(i,j)wv(i,j,n)$$

$$\sum_n d^k(s,n) + \textbf{slack}^k(s) \geq r(s)$$

Unsatisfied Demand

$$Tf^k(i,j,n) = Ts^k(i,j,n) + \alpha(i,j)wv(i,j,n) + \beta(i,j)b^k(i,j,n)$$

$$Ts^k(i,j,n+1) \geq Tf^k(i,j,n) - U(1-wv(i,j,n))$$

$$Ts^k(i,j,n) \leq H^k, \; Tf^k(i,j,n) \leq H^k$$

*Upper Partial Mean

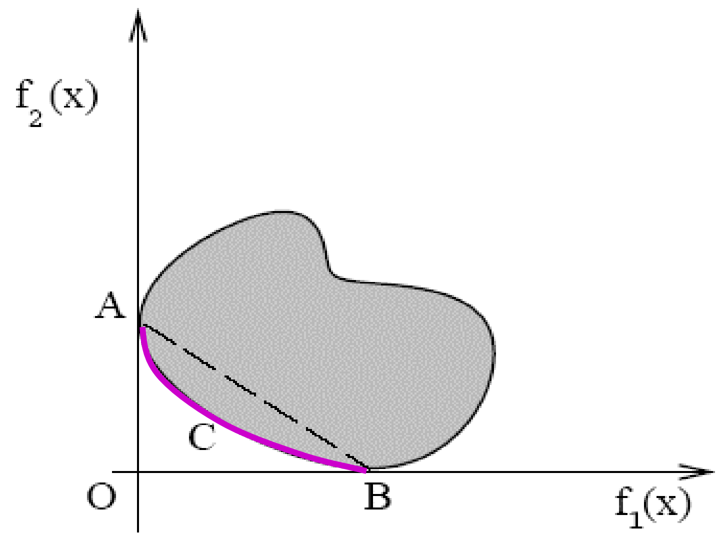
$$\Delta^k \geq H^k - \sum_k P^k H^k, \; \Delta^k \geq 0$$

* S.Ahmed and N. Sahinidis. *Robust process planning under uncertainty*. 1998

Multiobjective Optimization

$$\min_{x \in C} F(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_n(x) \end{pmatrix}$$

$$C = \{x : h(x) = 0,\ g(x) \le 0,\ a \le x \le b\}$$

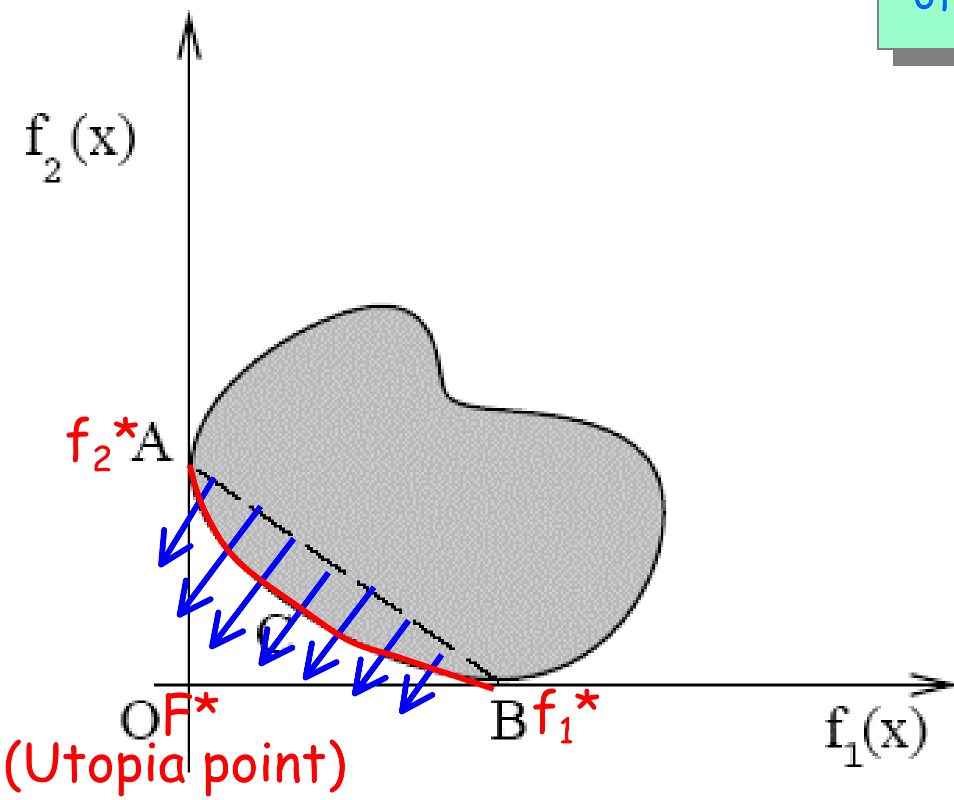


Pareto Optimal Solution:

A point $x^* \epsilon C$ is said to be Pareto optimal if and only if there is no such $x \epsilon C$ that $f_i(x) \le f_i(x^*)$ for all $i=\{1,2,\ldots,n\}$, with at least one strict inequality.

Normal Boundary Intersection (NBI)

$$\text{Min } F(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix}$$



Advantage: can produce a set of evenly distributed Pareto points independent of relative scales of the functions

NBIω:

$$\max_{x,t} \; t$$

$$\text{s.t. } \Phi\omega + t\,\hat{n} = F(x) - F^*$$

$$h(x) = 0$$

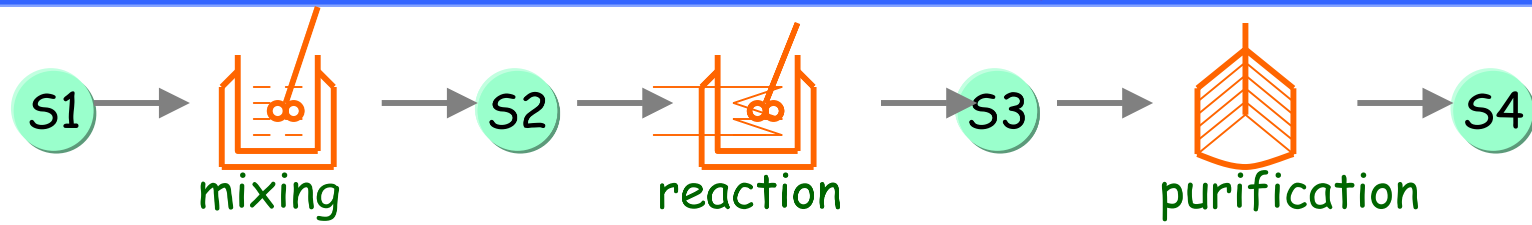
$$g(x) \le 0$$

$$a \le x \le b$$

A point in the Convex Hull of Individual Minima (CHIM)

* I. Das and J. Dennis. *NBI: A new method for generating the Pareto surface in nonlinear multicriteria optimization problems.* 1996

Case Study



maximize t

subject to $\sum_{(i,j)} wv(i,j,n) \leq 1$

$$st^k(s,n) = st^k(s,n-1) - d^k(s,n) + \sum \rho^P(s,i) \sum b^k(i,j,n-1) + \sum \rho^c \sum b^k(i,j,n)$$

$$st^k(s,n) \leq stmax(s)$$

$$Vmin(i,j)wv(i,j,n) \leq b^k(i,j,n) \leq Vmax(i,j)wv(i,j,n)$$

$$\sum d^k(s,n) + slack^k(s) \geq r(s)$$

$$Tf^k(i,j,n) = Ts^k(i,j,n) + \alpha(i,j)wv(i,j,n) + \beta(i,j)b^k(i,j,n)$$

$$Ts^k(i,j,n+1) \geq Tf^k(i,j,n) - U(1-wv(i,j,n))$$

$$Ts^k(i,j,n) \leq H^k,\ Tf^k(i,j,n) \leq H^k$$

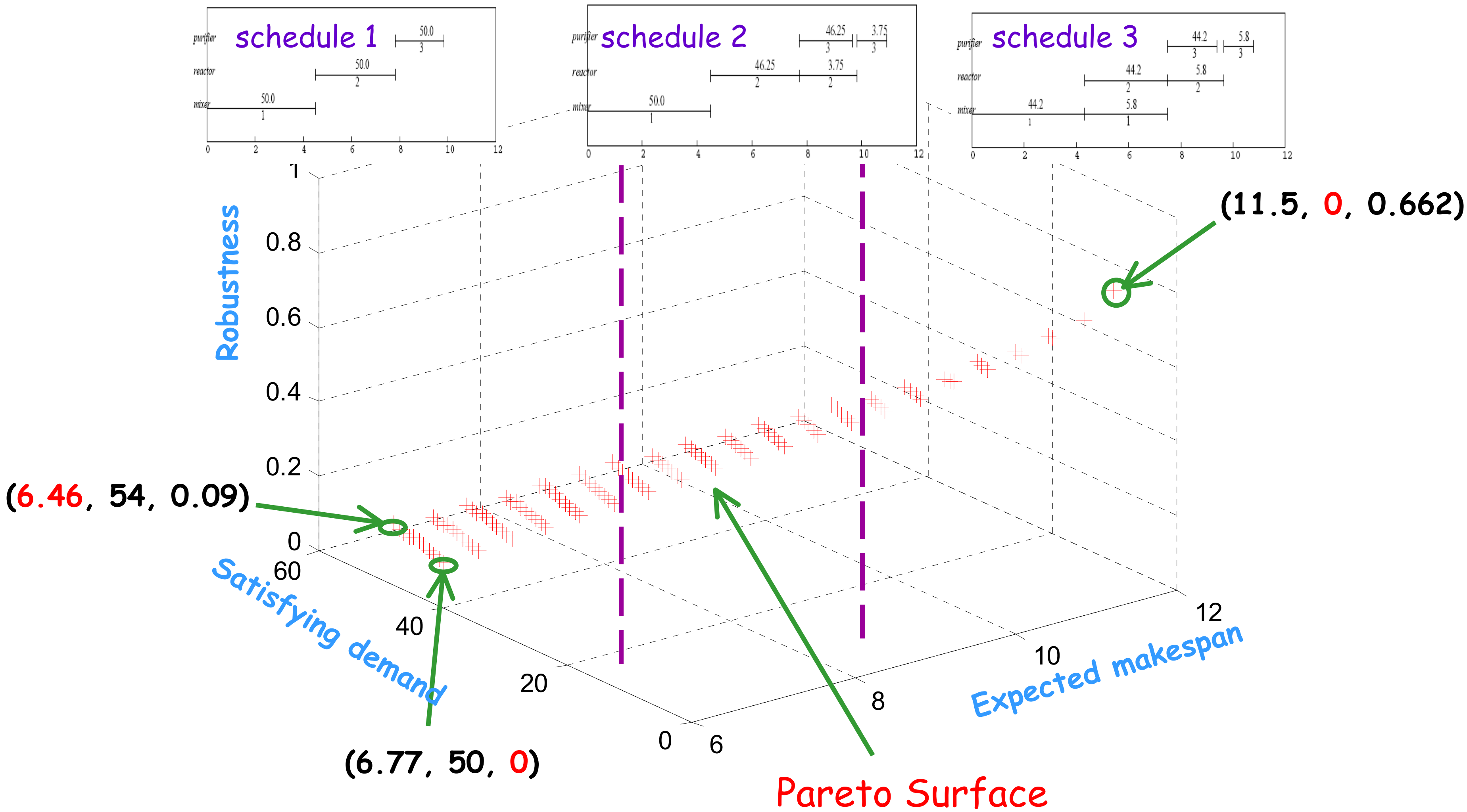
$$\Delta^k \geq H^k - \sum P^k H^k,\ \Delta^k \geq 0$$

$$f_1(x^*) = \begin{pmatrix} 6.46 \\ 54 \\ 0.09 \end{pmatrix} \quad f_2(x^*) = \begin{pmatrix} 11.5 \\ 0 \\ 0.66 \end{pmatrix} \quad f_3(x^*) = \begin{pmatrix} 6.77 \\ 50 \\ 0 \end{pmatrix}$$

$$F^* = \begin{pmatrix} 6.46 \\ 0 \\ 0 \end{pmatrix} \qquad \Phi = \begin{pmatrix} 0 & 4.14 & 0.31 \\ 54 & 0 & 50 \\ 0.09 & 0.66 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 4.14 & 0.31 \\ 54 & 0 & 50 \\ 0.09 & 0.66 & 0 \end{pmatrix} \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} = \begin{pmatrix} \sum_k P^k H^k - 6.46 \\ \sum_k P^k \sum_s slack^k(s) \\ \sum_k P^k \Delta^k \end{pmatrix}$$

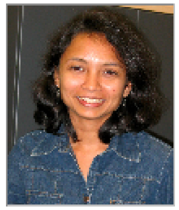
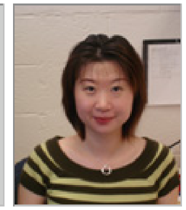
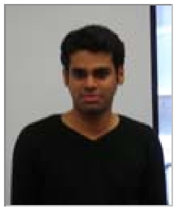
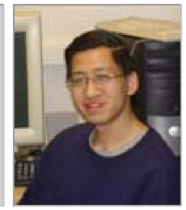
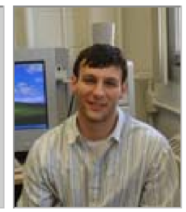
Case Study



schedule 1
schedule 2
schedule 3
Robustness
Satisfying demand
Expected makespan
(11.5, 0, 0.662)
(6.46, 54, 0.09)
(6.77, 50, 0)
Pareto Surface

Acknowledgements

Graduate Students

	Dan Wu		Ipsita Banerjee		Zhenya Jia
	Nripen Sharma (Co-advice Prof. M. Yarmush)		Patricia Portillo (Co-advice Prof. F.Muzzio)		Eddie Davis
	Ian Glasgow (Co-advice Prof. P.Stuart University of Montreal)		Hong Yang (Co-advice Prof. C. Roth)		Steve Guzikowski (Co-advice Prof. C. Roth)

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	Agib Pierre-Louis		Victor Low		

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