Progress and Challenges in Discrete and Continuous Optimization for Process Systems Engineering

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Center for Advanced Process Decision-making

Faculty

				
Larry Biegler	**Ignacio Grossmann**	**Nick Sahinidis**	**Jeffrey Siirola**	**Erik Ydstie**

PhD Students:	**26**	**MS Students:**	**7**
Post Docs:	**5**	**Visitors:**	**7**

Center for Advanced Process Decision-making

Goals:

1. Do basic research in Process Systems Engineering

2. Produce students with unique skills in PSE

3. Interact with industry through mutually beneficial projects

Basic methodologies	**Areas of application**
Process modeling	Process and product synthesis
Mathematical programming	Energy Systems
Systems Engineering	Supply chain optimization
Process control	Molecular Design
Advanced computing	Systems Biology

CAPD
Center for Advanced Process Decision-making

Industrial Partners

ABB	*GAMS*
Air Liquide	*NETL*
Air Products	*Neste Engineering Oy*
Bayer	*Nova Chemicals*
Braskem	*Paragon Decision*
Cognizant	*Petrobras*
Dow Chemical	*Pfizer*
Eastman Chemical	*PPG*
Ecopetrol	*Praxair*
ExxonMobil	*Total*
FICO	*Unilever*

Research Ignacio Grossmann

Mixed-Integer Programming

Global Optimization of Bilinear GDP Problems ***Juan Ruiz, Francisco Trespalacios***
Global Optimization of Multiperiod Blending ***Scott Kolodziej ExxonMobil***
Cyber-MINLP Virtual Environment ***Biegler, Margot, Ruiz, Sahinidis IBM-Lee, Waechter***
LOGMIP- ***Aldo Vecchietti, INGAR, Argentina***
GAMS based interfaces ***Rosanna Franco***

Process Synthesis/Energy

Optimal Design of IGCC Plants ***Ravi Kamath NETL****
Simultaneous Optimization, Heat Integration and Water Management ***LinlinYang NETL***
Optimal Design of Biofuel Plants ***Mariano Martin***
Optimal Integrated Water Process Networks in Biofuel Plants ***Elvis Ahmetovic***
Modeling and Optimization of Water Treatment Systems ***Berta Galan***

Research Ignacio Grossmann (cont)

Planning and Scheduling

Enterprise-wide Optimization *Biegler, Grossmann, Hooker, Secomandi, Snyder*
ABB, Air Products, Air Liquide, Dow Chemical, ExxonMobil, PPG, Praxair, NOVA, TOTAL, Unilever

Multistage Stochastic Optimization of Offshore Facilities *Vijay Gupta ExxonMobil*
Design of Responsive and Uncertain Supply Chains *Fengqi You*
Optimal Capacity Planning under Uncertain Electricity Prices *Sumit Mitra, Praxair*
Optimal Design of Reliable Integrated Sites *Sebastian Terrazas Pablo Garcia Herrero Dow Chemical*
Optimal Multisite Planning and Scheduling *Bruno Calfa Dow Chemical*
Optimal Scheduling of Crude Oil Operations *Sylvain Mouret TOTAL*
Optimal Model-Based Refinery Planning *Abdulah Alattas BP*
Planning and long-term scheduling for PPG glass production*Ricardo Lima PPG*
Batch Process Scheduling under Electricity Price Constraints *Pedro Castro ABB*

Motivation discrete and continuous optimization

Cost and inventory reductions, reducing energy, water consumption, and investment in energy systems, improving responsiveness., global optimization of energy potentials

Discrete and continuous optimization models

Provide a powerful framework for modeling selection of:

a) **Structure of system**
b) **Design parameters**

Models

a) **Mixed-integer linear programming (MILP)**
b) **Mixed-integer nonlinear programming (MINLP)**
c) **Generalized Disjunctive Programming (GDP/linear-nonlinear)**

Goal: Overview state-of-art, progress and future directions:

a) **What tools are available for effectively *solving linear and nonlinear discrete/continuous models*?**

b) **What are major challenges for *global optimality and handling uncertianty?***

Mathematical Programming

MINLP: ***Mixed-integer nonlinear programming***

$$\min Z = f(x, y)$$
$$s.t. \quad h(x, y) = 0$$
$$g(x, y) \le 0$$
$$x \in R^n, \quad y \in \{0,1\}^m$$

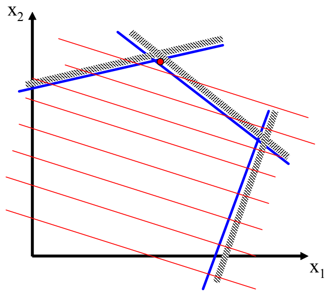
$$f(x): R^n \rightarrow R^1, h(x): R^n \rightarrow R^m, g(x): R^n \rightarrow R^q$$

MILP: *f, h, g* linear

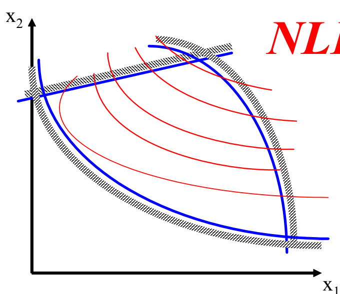
LP: *f, h, g* linear, only *x*

NLP: *f, h, g* nonlinear, only *x*

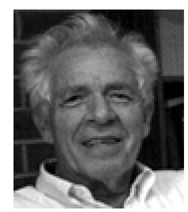
Evolution of Mathematical Programming

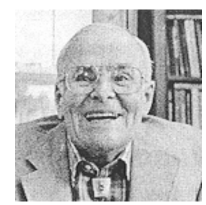


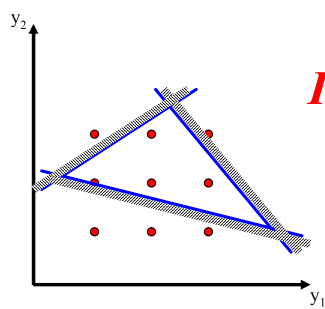
LP: Linear Programming ***Kantorovich (1939), Dantzig (1947)***



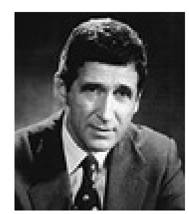
NLP: Nonlinear Programming ***Karush (1939); Kuhn, A.W.Tucker (1951)***







IP: Integer Programming ***R. E. Gomory (1958)***



Major developments in last 20 years

- **Interior Point Method for LP** ***Karmarkar (1984)***

- **Convexification of Mixed-Integer Linear Programs**
  Lovacz & Schrijver (1989), Sherali & Adams (1990),
  Balas, Ceria, Cornuejols (1993)

- **Modeling Systems** **GAMS, AMPL, AIMMS**

- **MILP codes:** **CPLEX, GUROBI, XPRESS**

- **NLP codes:** **MINOS, CONOPT, SNOPT, IPOPT**

- **MINLP** ***Duran & Grossmann (1986)***

- **Global Optimization** ***Floudas(1990), Sahinidis (1996)***

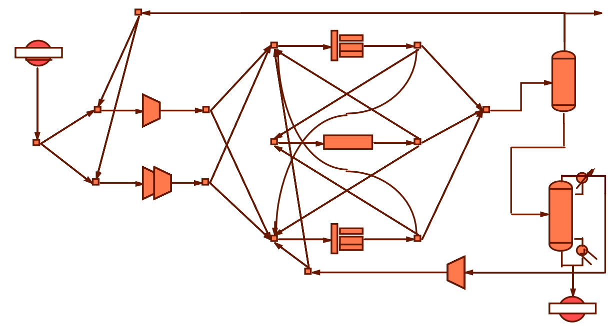
- **Logic-based optimization** ***Hooker (1991), Raman & Grossmann (1994)***

- **Hybrid-systems** ***Barton & Pantelides (1994), Bemporad & Morari (1998)***

Applications of Mathematical Programming in Chemical Engineering

Process Design

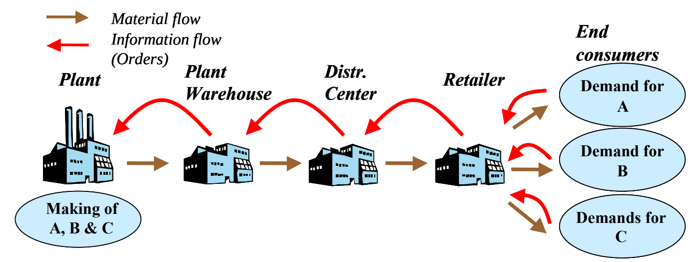
Process Synthesis



Production Planning

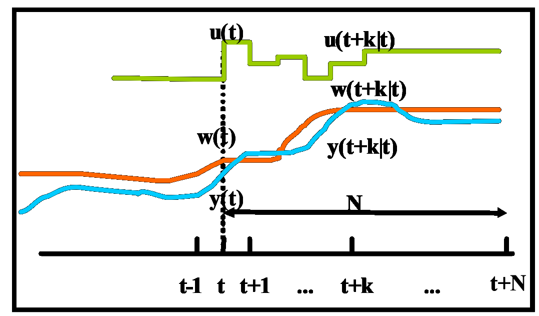
Process Scheduling

Supply Chain Management



Process Control

Parameter Estimation



LP, MILP, NLP, MINLP, Optimal Control

Major contribution: new problem representations and models

MILP

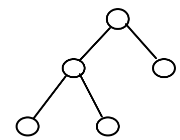
$$\min Z = a^T y + b^T x \qquad \textit{Objective function}$$

$$st \qquad Ay + Bx \leq d \qquad \textit{Constraints}$$

$$y \in \{0,1\}^m, \; x \geq 0$$

Cutting planes *Gomory (1959)*

Branch and Bound *Beale (1958), Balas (1962), Dakin (1965)*



LP (simplex) based

Theory for Convexification

Lovacz & Schrijver (1989), Sherali & Adams (1990),

Balas, Ceria, Cornuejols (1993)

Branch and cut *Johnson, Nemhauser & Savelsbergh (2000)*

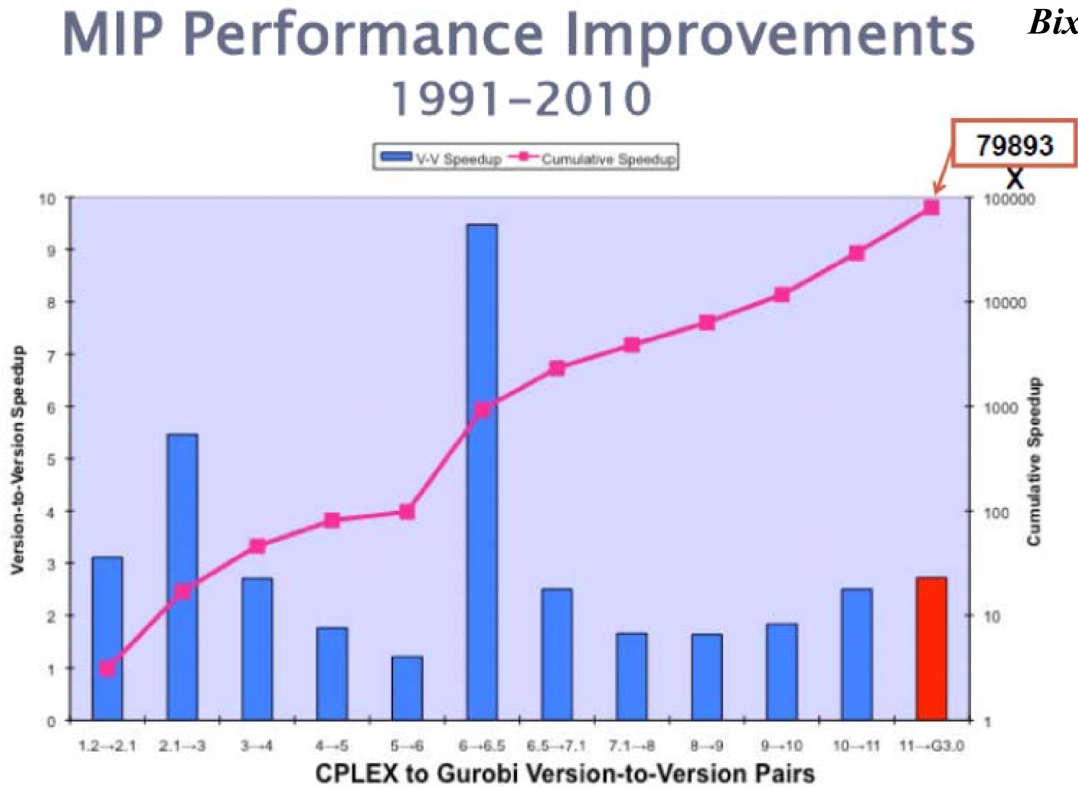
Combine Branch and Bound with Cutting Planes

Codes: CPLEX, XPRESS, GUROBI

Algorithmic features: Cuts, presolve, heuristics, multithread

Progress in Mixed-Integer Linear Programming

Bixby, Rothberg and Gu (2009)



=> <u>**80,000 speed-up!!**</u>

CPLEX 1.2 to Gurobi 3.0

Unit-Commitment Model: California 7-Day Model
2,856 0-1 vars, 22,899 cont vars, 48,939 constr.

1999 CPLEX 7.0: 1 hr initial LP, unfinished after 8 hours
2010 Gurobi 3.0: ~3 min *(195 secs)* to optimality!

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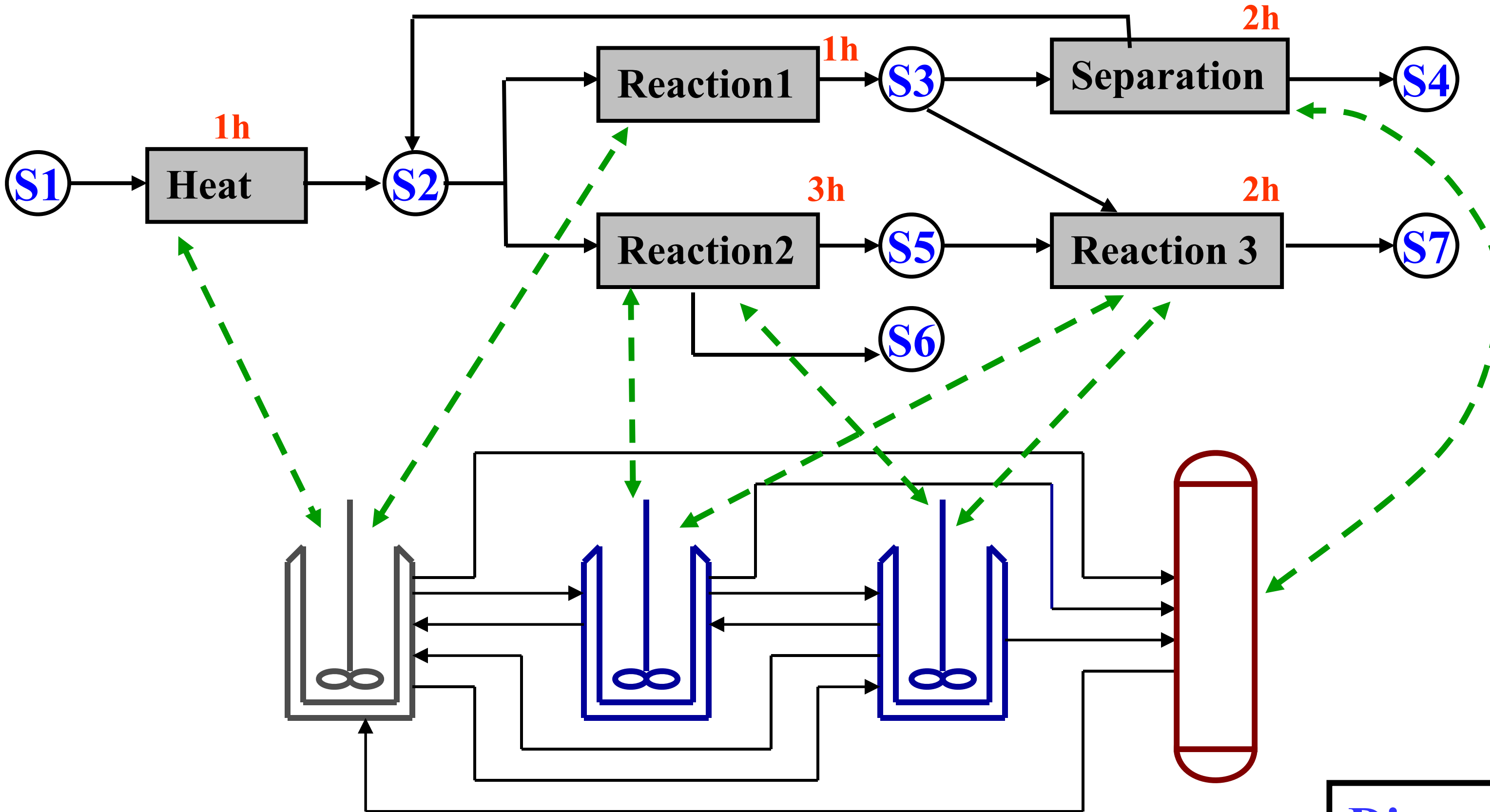
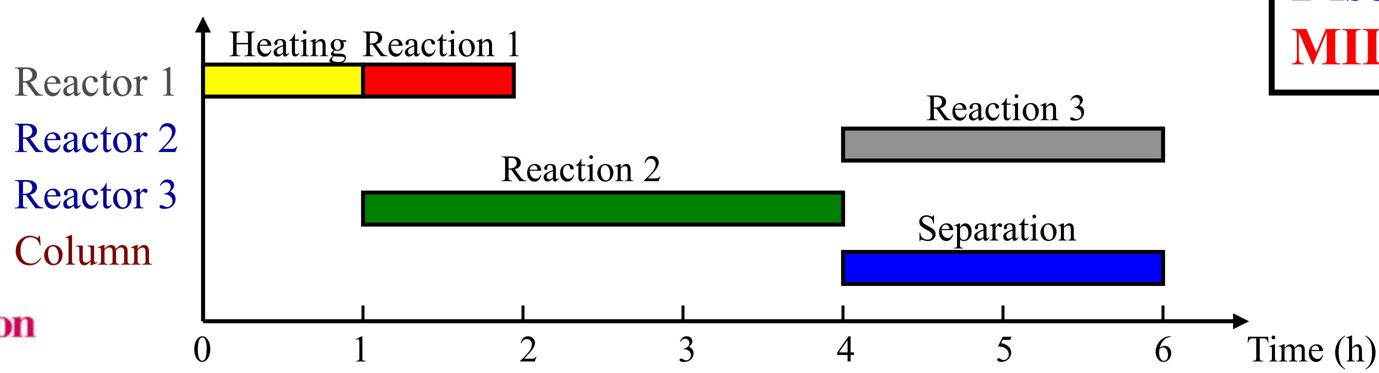
Which Single Feature Helps Most?

(After CPLEX 6.5 < 1000 seconds, Before CPLEX 6.5 unsolvable)

Cuts	53.7x
Presolve	10.8x
Variable selection	2.9x
No heuristics	1.4x
No node presolve	1.3x

State Task Network (STN) *(Kondili, Pantelides, Sargent, 1993)*





Discrete time
MILP model

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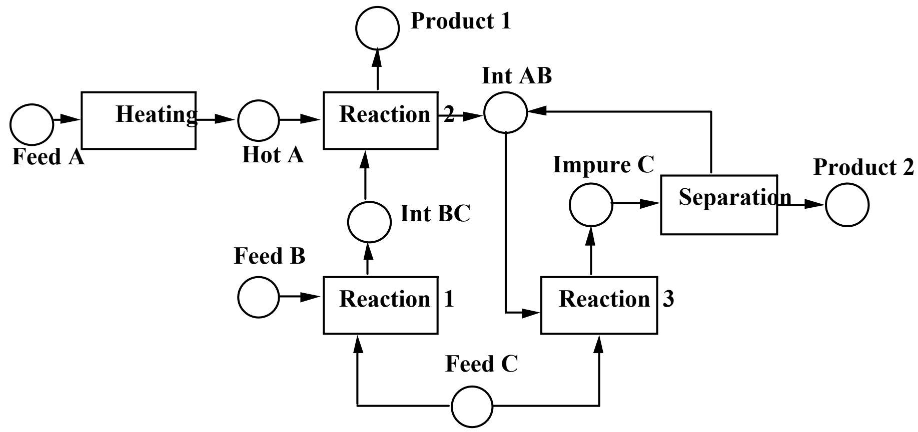
Classical Kondili Example

STN



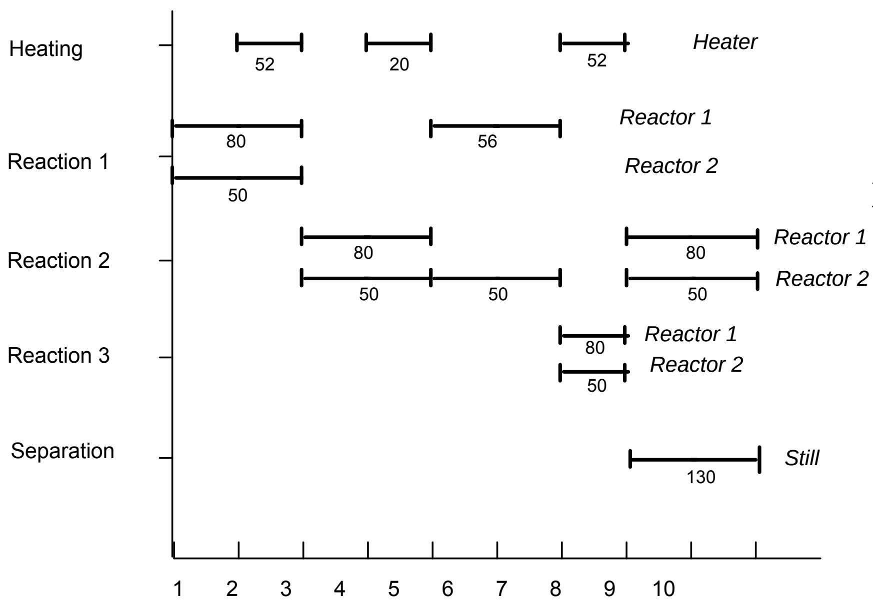
MILP

72 0-1 variables

179 continuous variables

250 constraints

Optimal Schedule



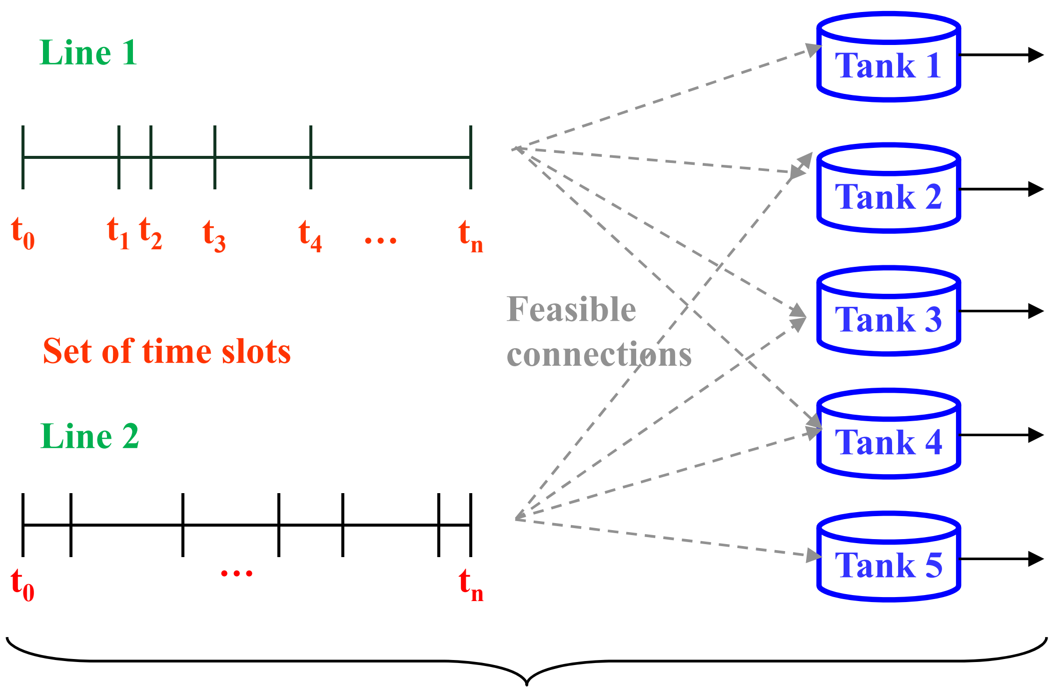
1987 Kondili's B&B: 908 sec, 1466 nodes, ***Vax-8600***

1992 Shah's B&B: 119 sec, 419 nodes, ***SUN Sparc***

2011 CPLEX 12.1: 0.2 sec!! 14 nodes!! ***Lenovo-T60***

Tank Farm Optimization Problem

Terrazas-Moreno, Wassick, Grossmann (2011)



Multi-operation Sequencing[1] (MOS) model for scheduling of production orders:

- Slot-based continuous time model

Given

- **A set of orders**
- **A set of production lines**
- **A set of tanks**
- **Release and due dates for production orders**
- **A set of shipping resources**
- **Intervals where those shipping resources are available**

Determine:

- **Schedule of production orders**
- **Assignment of products to tanks**

With the objective of:

- **Maximizing allocated product**

2 lines, 10 tanks, 21 orders (8 products) 4 weeks

MILP: 1,340 0-1 vars, 16,561 cont vars, 40,261 constraints 530 s CPUtime Gurobi 4.0

(1) Mouret. S., Grossmann I.E., Pestiaux P. (2010)

Nonlinear Programming

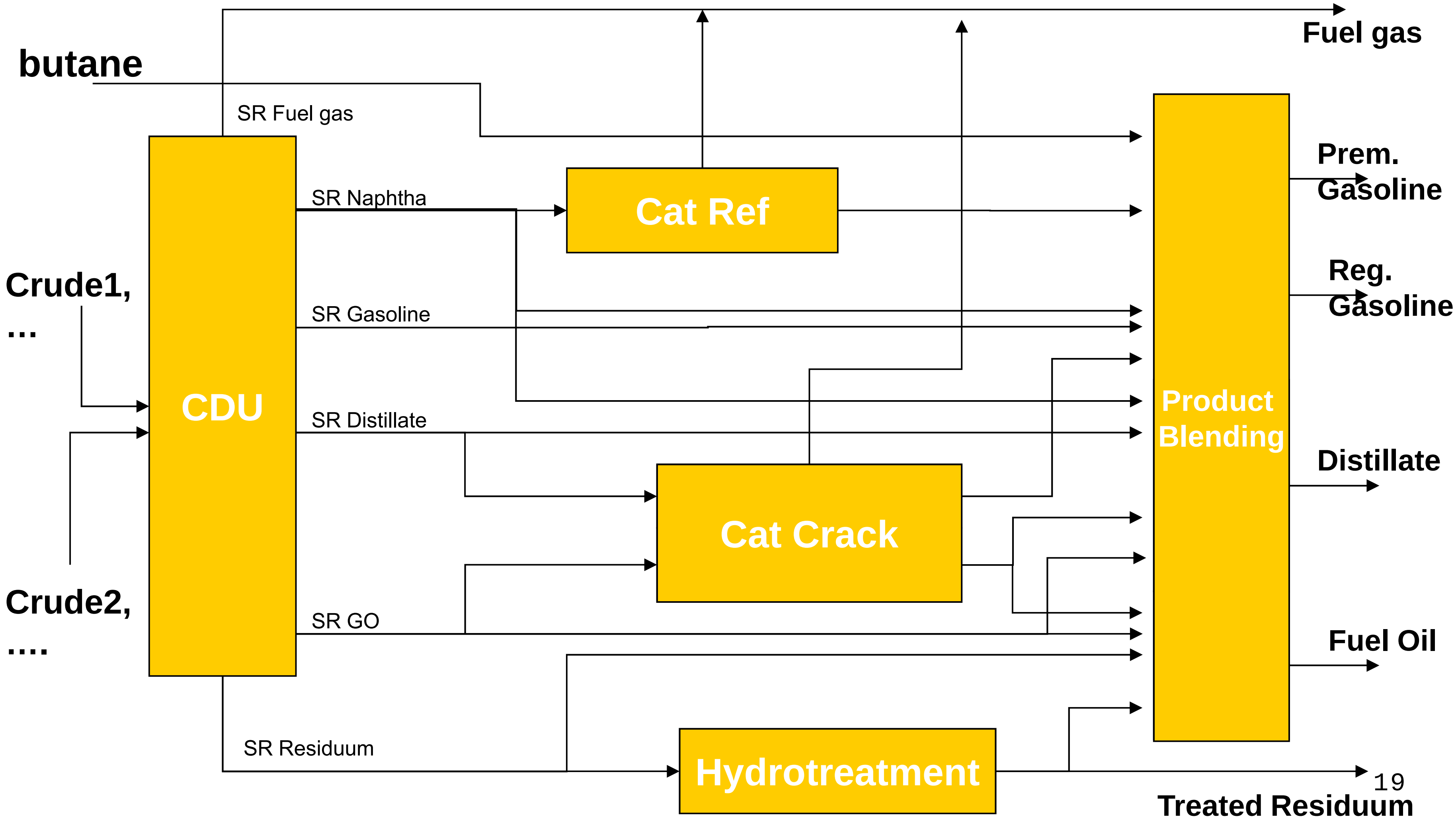
NLP: Algorithms *(variants of Newton's method)*

- Sucessive quadratic programming (SQP) *(Han 1976; Powell*
- Reduced gradient
- Interior Point Methods

Nonlinear CDU Models in Refinery Planning Optimization

Alattas, Palou-Rivera, Grossmann (2010)

Typical Refinery Configuration *(Adapted from Aronofsky, 1978)*



Planning Model Example Results

Crude1	Louisiana	Sweet	Lightest
Crude2	Texas	Sweet	
Crude3	Louisiana	Sour	
Crude4	Texas	Sour	Heaviest

- Comparison of *nonlinear fractionation index (FI)* with *linear* fixed yield (FY) and swing cut (SC) models
- Economics
  - FI calculates the maximum profit scenario

Model	Case1	Case2	Case3
FI	245	249	247
SC	195	195	191
FY	51	62	59

MINLP

Mixed-Integer Nonlinear Programming

$$\min Z = f(x,y)$$
$$s.t. \quad h(x,y)=0$$
$$g(x,y) \le 0$$
$$x \in X, \; y \in Y$$
$$X = \{x \mid x \in R^n, x^L \le x \le x^U, Bx \le b\}$$
$$Y = \{y \mid y \in \{0,1\}^m, Ay \le a\}$$
$$f(x): R^n \to R^1, h(x): R^n \to R^m, g(x): R^n \to R^q$$

Remarks

1. **Basic MINLP algorithms rely on convexity assumptions**
2. **When applied to nonconvex problems suboptimal solutions may be obtained**

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Mixed-integer Nonlinear Programming

Algorithms

Branch and Bound (BB) ***Ravindran and Gupta (1985), Stubbs, Mehrotra (1999), Leyffer (2001)***

Generalized Benders Decomposition (GBD) ***Geoffrion (1972)***

Outer-Approximation (OA) ***Duran and Grossmann (1986), Fletcher and Leyffer (1994)***

LP/NLP based Branch and Bound ***Quesada, Grossmann (1994)***

Extended Cutting Plane(ECP) ***Westerlund and Pettersson (1992)***

GAMS

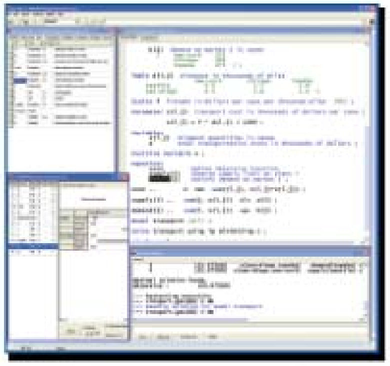
Optimization

www.gams.com

- Support
- Sales
- Solvers
- Documentation
- Model Library
- gamsworld.org

High-Level Modeling

The General Algebraic Modeling System (GAMS) is a **high-level modeling system** for mathematical programming problems. GAMS is tailored for complex, large-scale modeling applications, and allows you to build large maintainable models that can be adapted quickly to new situations. Models are **fully portable** from one computer platform to another.



GAMS Integrated Developer Environment for editing, debugging and solving models and viewing data.

Wide Range of Model Types

GAMS allows the formulation of models in **many different problem classes**, including

- Linear (LP) and Mixed Integer Linear (MIP)
- Quadratic Programming (QCP) and Mixed Integer QCP (MIQCP)
- Nonlinear (NLP) and Mixed Integer NLP (MINLP)
- Constrained Nonlinear Systems (CNS)
- Mixed Complementary (MCP)
- Programs with Equilibrium Constraints (MPEC)
- Conic Programming Problems
- Stochastic Linear Problems

State-of-the-Art Solvers

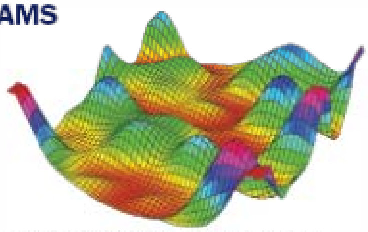
GAMS incorporates all major commercial and academic **state-of-the-art solution technologies** for a broad range of problem types, including global nonlinear optimization solvers.

MINLP and Global Solvers in GAMS

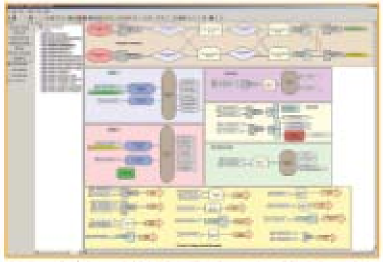
The area of Mixed Integer Nonlinear Programming (MINLP) and Global Optimization has experienced significant growth in industry and academia over the last years. More and more general purpose solution algorithms have been implemented and have matured into reliable solution systems:

- **AlphaECP**[Δ]: Extended cutting plane method from Åbo Akademi University, Finland
- **BARON**: Branch-And-Reduce Optimization Navigator for proven global solutions from The Optimization Firm
- **Bonmin**[Δ]: Hybrid outer-approximation based branch-and-cut algorithm jointly developed by a collaboration between Carnegie Mellon University and the IBM Corporation and distributed from COIN-OR
- **DICOPT**: Outer approximation framework from Carnegie Mellon University
- **LGO**: Lipschitz global optimizer from Pinter Consulting Services, Inc.
- **LINDOGlobal**[Δ]: A branch-and-bound solver for proven global solutions from Lindo Systems, Inc.
- **MSNLP/OQNLP**: Multi-start method for global optimization from Optimal Methods, Inc.
- **SBB**: Branch-and-Bound algorithm from ARKI Consulting & Development A/S

[Δ] New in GAMS 22.5.



Surface of a function with multiple local optima.
© Janos D. Pinter, PCS Inc.



Screenshot from SCMart Suite deploying MINLP models from Optience Corp.

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Username
Password
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Home | Goals | Participants | Instructions | Contribute Problems | Open Problems | Libraries of Problems | Forum | Resources

CMU-IBM Cyber-Infrastructure for MINLP collaborative site

This collaborative site has as a major goal to promote the optimization of linear and nonlinear models with one or several alternative model formulations involving discrete and continuous variables through mixed-integer nonlinear programming (MINLP), or generalized disjunctive programming (GDP). Three major objectives are:

- Create a library of optimization problems that can be generally formulated as MINLP/GDP models.
- Provide high level descriptions of the problems with one or several model formulations with corresponding input files for one or several instances.
- Allow users to pose open problems that are unsolved and with unknown or tentative formulations

$$\min Z = f(x,y)$$
$$s.t. \quad g(x,y) \le 0$$
$$x \in X,\ y \in Y$$

We invite researchers and practitioners to contribute to the library of problems and models, and to participate in the discussions on these problems. We look forward to collaborating with you!

About us

- Goals of our project
- Participants of the project

Contribute

- Create an account
- Learn how to contribute problems
- Contribute solved problems, models, and instanes to our library
- Post open unsolved problems

Our library

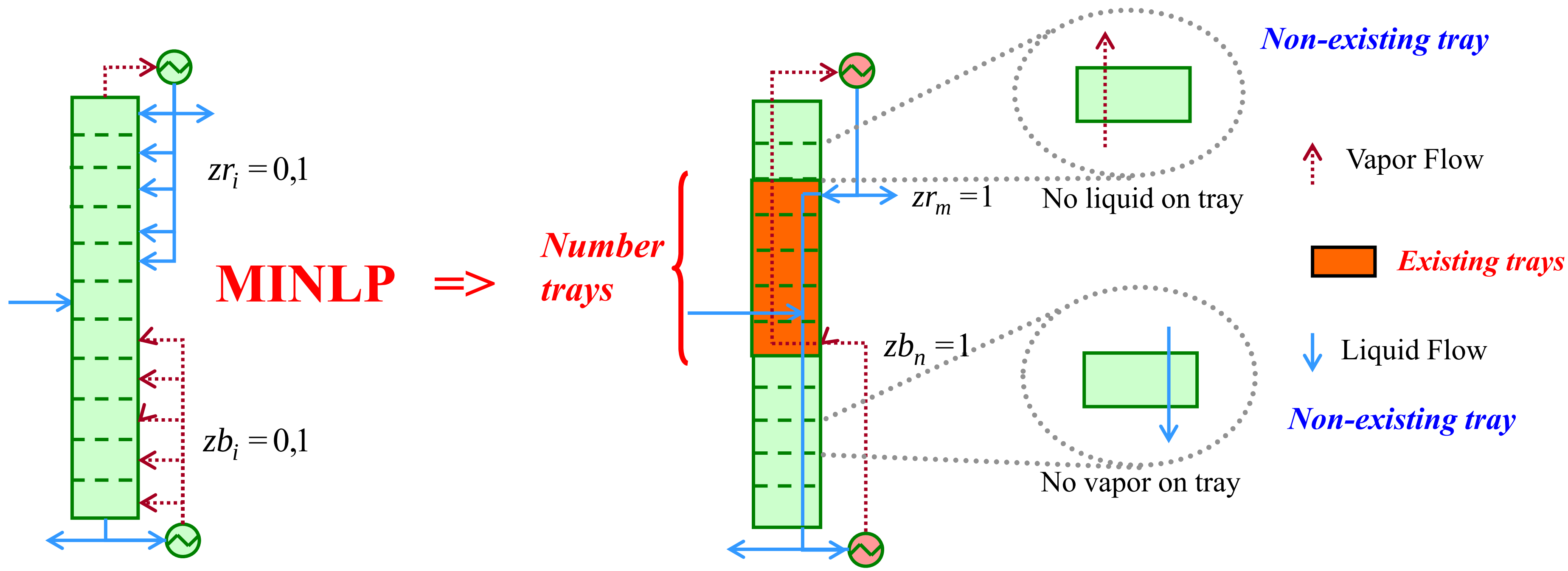
- View our library of problems
- Discuss problems in the forums

Resources

- Conferences
- Lectures and Tutorials

Optimization of Number of Trays

Viswanathan & Grossmann (1993)



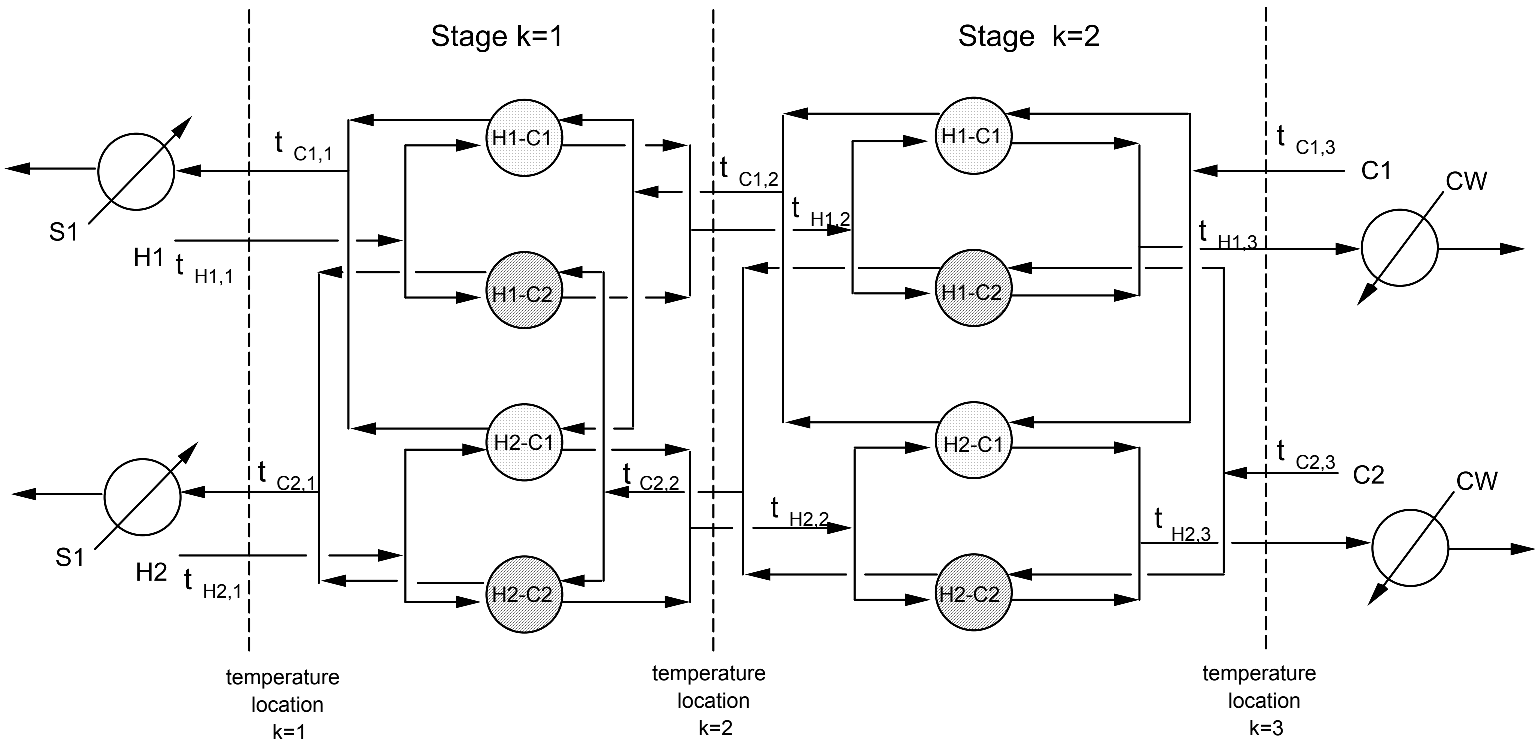
Discrete variables: **Number of trays, feed tray location.**

Continuous variables: **reflux ratio, heat loads, exchanger areas, column diameter.**

Acetone-acetonitrile-water, max 25 trays, Virial-UNIQUAC
MINLP: 22 0-1 vars, 891 cont, vars, 957 const. ~ 40 min

Synthesis of Heat Exchanger Networks

Yee and Grossmann (1990)

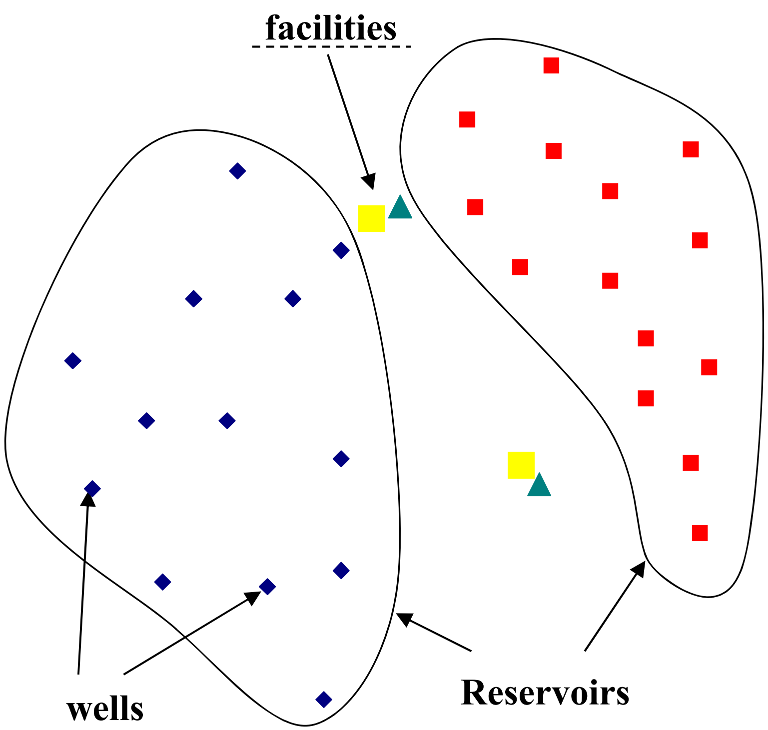


Multiple stages with potential heat exchangers $z_{ijk} = 0,1$

> *7 hot, 3 cold streams*
> **MINLP 115 0-1, 447 cont vars, 476 constr. 26s CPU-time** *(DICOPT-2011)*

Optimal Development of Oil Fields *(deepwater)*

Offshore field having several reservoirs (oil, gas, water)



Gupta, Grossmann (2011)

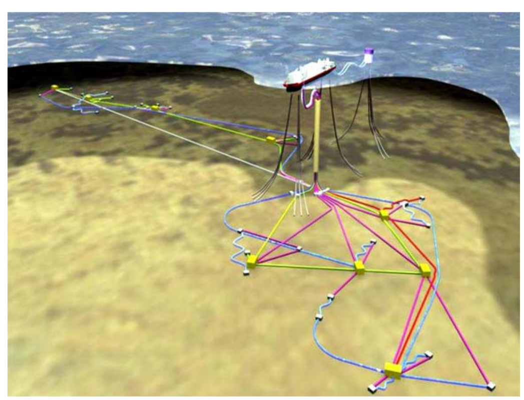
Decisions:

- ➢Number and capacity of FPSO facilities
- ➢Installation schedule for facilities
- ➢Number of sub-seawells to drill
- ➢Oil/gas production profile over time

Objective:

➢**Maximize the Net Present Value (NPV) of the project**

FPSO ***(Floating Production Storage Offloading)***



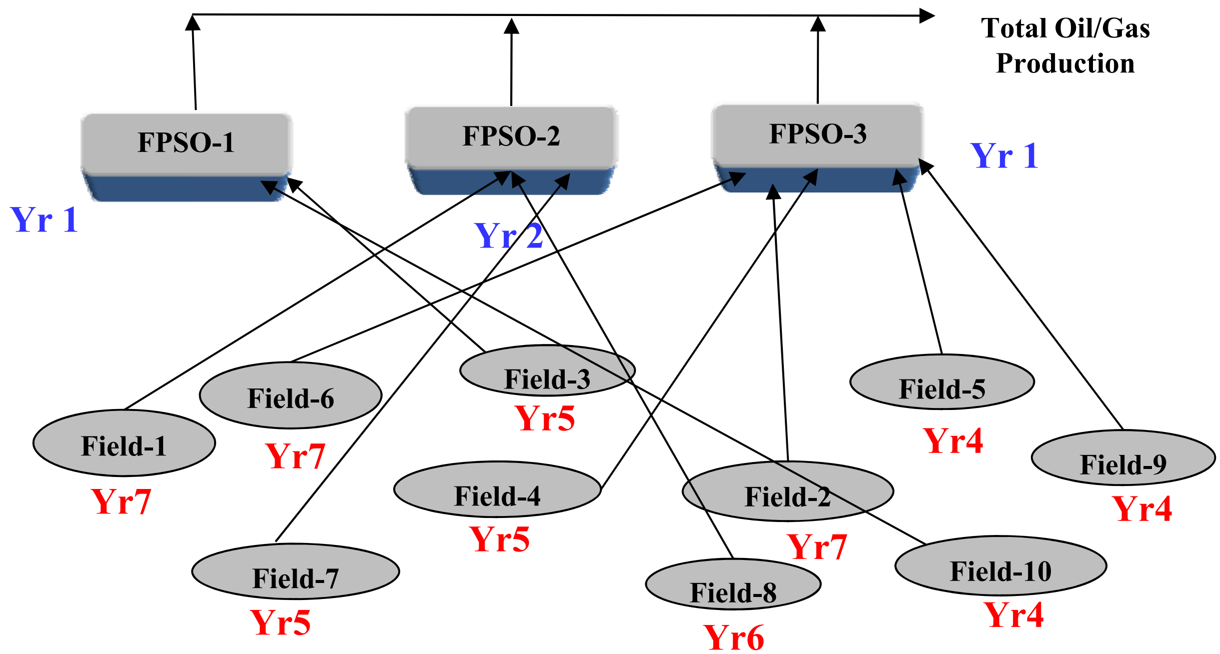
MINLP model

- **Nonlinear reservoir behavior**
- **Three components (oil, water, gas)**
- **Lead times for FPSO construction**
- **FPSO Capacity expansion**
- **Well Drilling Schedule**

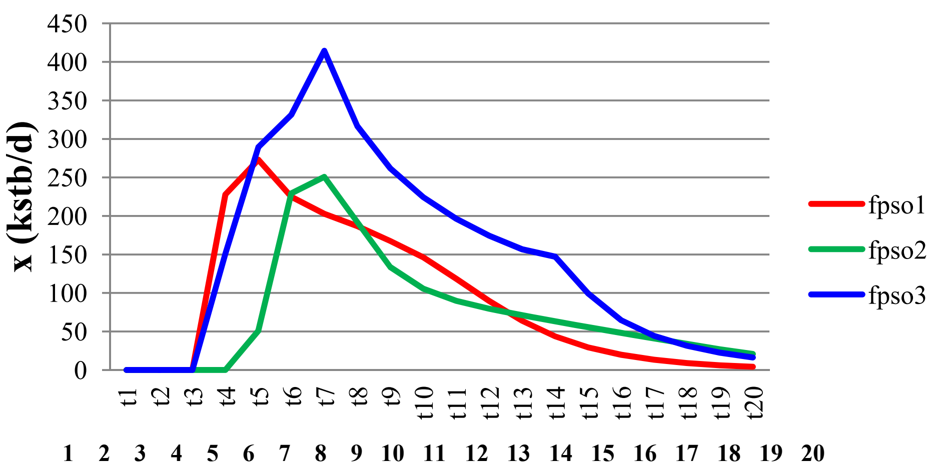
Example

Optimal NPV = *$30.946 billion*

20 Year Time Horizon
10 Fields
3 FPSOs
23 Wells
3 Yr lead time FPSO
1 Yr lead time expansion



Oil Flowrate



Computational performance

MINLP can be reformulated as MILP using exact linearization and piece-wise linearization approximation

	MINLP
Discrete Var.	483
SOS1 Var.	0
Continuous Var.	5,684
Constraints	9,877
Solver	DICOPT 2x-C
NPV (billion dollars)	30.946
CPU time(s)	**67**

**Solved in GAMS 23.6.3 on an Intel Core i7 machine with 4 GB of RAM*

=> MINLP model basis for Stochastic Programming

Simultaneous Cyclic Scheduling and Control of a Multiproduct CSTR Reactor

Antonio Flores (U. Iberoamericana)

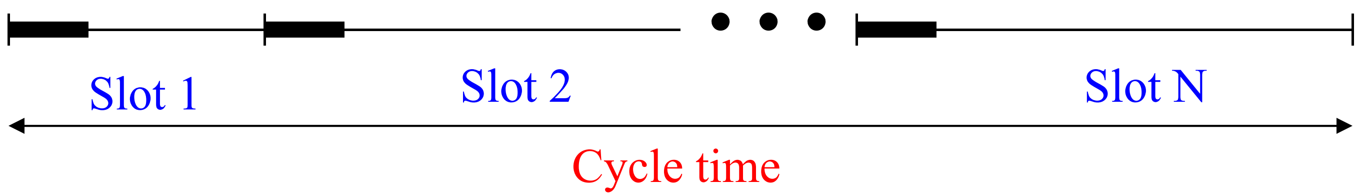
Given is a CSTR reactor
- **N products**
- **Lower bounds demand rates**
- **Dynamic model for reactions**

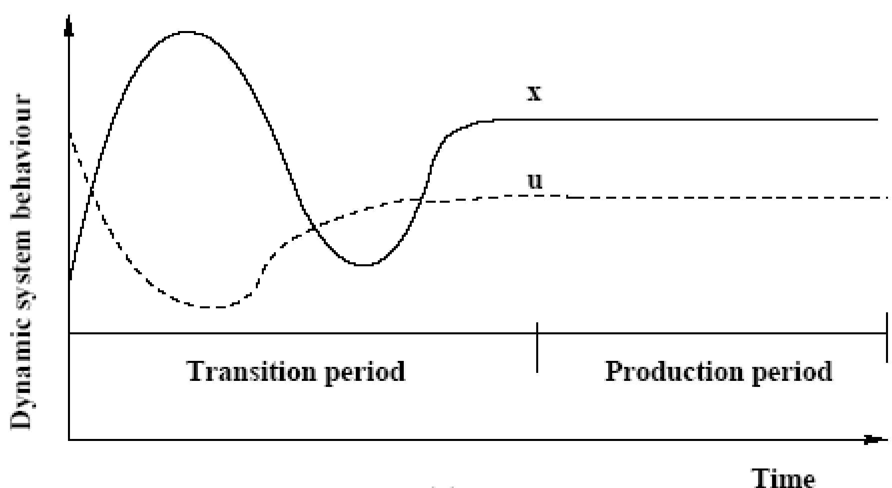
Determine cyclic schedule
- **Cycle time**
- **Sequence**
- **Amounts to produce**
- **Lenghts transitions and their dynamic profile**

Objective: Maximize total profit

Basic ideas MIDO model

$$y_{il} = \begin{cases} 1 & product\ i\ assigned\ slot\ l \\ 0 & otherwise \end{cases}$$





(b)

Requires guessing transition times

Use orthogonal collocation for converting dynamic eqtns into algebraic eqtns.

Discretized DAE solved as MINLP (DICOPT)

MIDO Optimization model

$$\max \quad \left\{ \sum_{i=1}^{N_p} \frac{C_i^p W_i}{T_c} - \sum_{i=1}^{N_p} \frac{C_i^s (G_i - W_i)}{2\Theta_i T_c} - \sum_{k=1}^{N_s} \sum_{f=1}^{N_{fe}} h_{fk} \sum_{c=1}^{N_{cp}} \frac{C^r t_{fck} \Omega_{c,N_{cp}}}{T_c} \left((x_{fck}^1 - \bar{x}_k^1)^2 + \ldots + (x_{fck}^n - \bar{x}_k^n)^2 + (u_{fck}^1 - \bar{u}_k^1)^2 + \ldots + (u_{fck}^m - \bar{u}_k^m)^2 \right) \right\} \quad (1)$$

s.t. Scheduling constraints:

Product assignments
Amounts manufactured
Processing times
Transition constraints
Timing relations

Dynamic and control optimization

Dynamic mathematical model discretization
Continuity constraint between finite elements
Model behavior at each collocation point

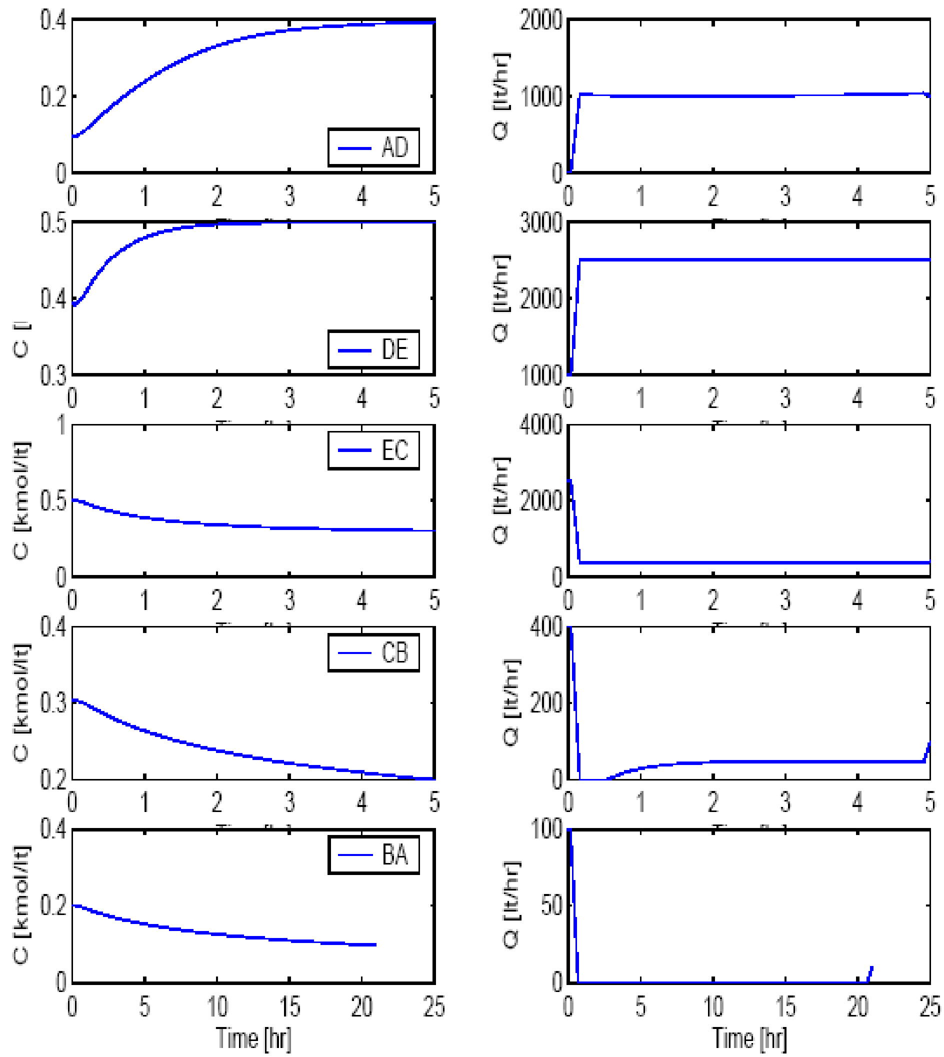
Reformulated as MINLP

Example: 5 products

Results

Slot	Product	Process time [h]	Production rate [Kg/h]	w [Kg]	Transition Time [h]	T start [h]	T end [h]
1	A	41.5	9.033	374.31	5	0	46.4
2	D	2.06	607	1249.4	5	46.4	53.6
3	E	23.4	1250	29270.4	5	53.6	82
4	C	4.48	278.72	1249.4	5	82	91.5
5	B	12.48	80	999.5	21	91.5	125

Product	Q [lt/hr]	C_R [mol/lt]	Demand rate [Kg/h]	Product cost [$/kg]	Inventory cost [$]
A	10	0.0967	3	200	1
B	100	0.2	8	150	1.5
C	400	0.3032	10	130	1.8
D	1000	0.393	10	125	2
E	2500	0.5	10	120	1.7



Optimal sequence

A→E→C→D→B→

Cycle time = 124.8 h

Profit = $7889/h

Generalized Disjunctive Programming (GDP)

Raman and Grossmann (1994) *(Extension Balas, 1979)*

Motivation: Facilitate modeling discrete/continuous problems

$$\min \; Z = \sum_k c_k + f(x)$$ **Objective Function**

$$s.t. \quad r(x) \le 0$$ **Common Constraints**

OR operator ⟶
$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \le 0 \\ c_k = \gamma_{jk} \end{bmatrix} \quad k \in K$$
Disjunction
Constraints
Fixed Charges

$$\Omega(Y) = true$$ **Logic Propositions**

$$x \in R^n, c_k \in R^1$$ **Continuous Variables**

$$Y_{jk} \in \{ true, \; false \}$$ **Boolean Variables**

$$f(x): R^n \to R^1, r(x): R^n \to R^m, g(x): R^n \to R^q$$

Properties: a) Every GDP can be transformed into an MINLP
b) Every bounded MINLP can be transformed into GDP

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Methods Generalized Disjunctive Programming

GDP

- **Logic based methods**
  - **Branch and bound**
    (Lee & Grossmann, 2000)
  - **Decomposition**
    Outer-Approximation
    Generalized Benders
    (Turkay & Grossmann, 1997)
- **Reformulation MINLP**
  Outer-Approximation
  Generalized Benders
  Extended Cutting Plane
  - **Convex-hull**
    Cutting plane
    (Sawaya & Grossmann, 2004)
  - **Big-M**

Big-M MINLP (BM)

- **MINLP reformulation of GDP**

$$\min Z = \sum_{k \in K} \sum_{j \in J_k} \gamma_{jk} \lambda_{jk} + f(x)$$

$$s.t. \quad r(x) \le 0$$

$$g_{jk}(x) \le M_{jk}(1 - \lambda_{jk}) \quad , j \in J_k, k \in K$$

$$\sum_{j \in J_k} \lambda_{jk} = 1, \quad k \in K$$

$$A\lambda \le a$$

$$x \ge 0,$$

Big-M Parameter

Logic constraints

Williams (1990)

NLP Relaxation $0 \le \lambda_{jk} \le 1$ **=> Lower bound to optimum of GDP**

Hull Relaxation Problem (HRP)

HRP:

$$\min Z = \sum_{k\in K}\sum_{j\in J_k}\gamma_{jk}\lambda_{jk} + f(x)$$

$$s.t. \quad r(x)\le 0$$

$$x = \sum_{j\in J_k}\nu^{jk}, k\in K$$

Disaggregated variables

$$0\le \nu^{jk}\le \lambda_{jk}U_{jk}, j\in J_k, k\in K$$

$$\sum_{j\in J_k}\lambda_{jk} = 1, k\in K$$

Convex Hull each disjunction

Perspective function

$$\lambda_{jk}g_{jk}(\nu^{jk}/\lambda_{jk})\le 0, \quad j\in J_k, k\in K$$

$$A\lambda\le a$$

Logic constraints

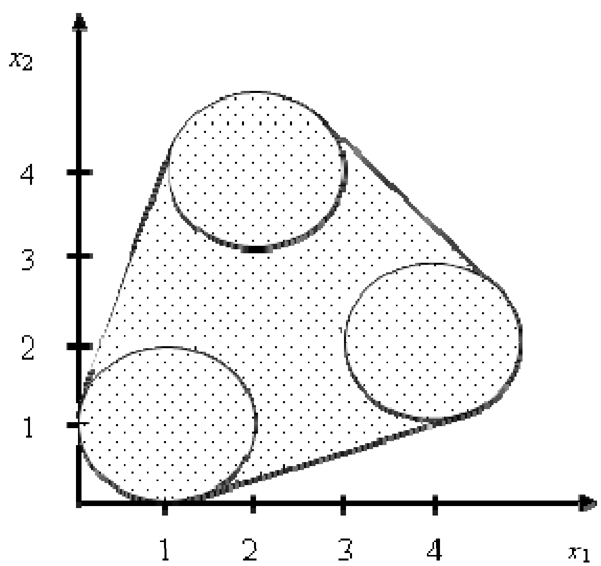
$$x, \nu^{jk}\ge 0, \; 0\le\lambda_{jk}\le 1, \; j\in J_k, k\in K$$

- **Property**: *The NLP (HRP) yields a lower bound to optimum of (GDP).*

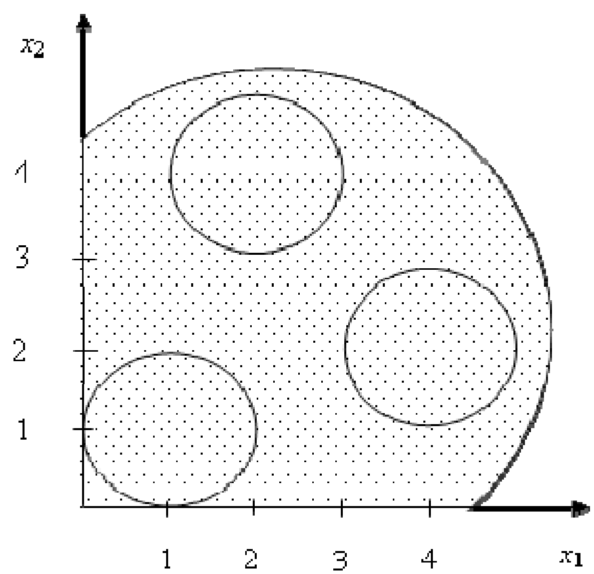
Strength Lower Bounds

- **Theorem 1**: ***The relaxation of (HRP) yields a lower bound that is greater than or equal to the lower bound that is obtained from the relaxation of problem (BM***

Grossmann, Lee (2003)



Convex hull relaxation



Big-M relaxation

Convex Hull of a set of disjunctions is smallest convex set that includes set of disjunctions.
Projected relaxation of (CH) onto the space of (BM) is as tight or tighter than that of (BM)

Multiperiod Production Planning LP Model

Fixed price purchases

$$Max\ PROFIT = \sum_{j\in J}\sum_{t\in T}\psi_{jt}S_{jt} - \sum_{j\in J}\sum_{t\in T}\phi_{jt}P_{jt}$$
$$-\sum_{i\in I}\sum_{j\in JM_i}\sum_{t\in T}\delta_{it}W_{ijt} - \sum_{j\in J}\sum_{t\in T}\xi_{jt}V_{jt} - \sum_{j\in J}\sum_{t\in T}\theta_{jt}SF_{jt}$$

Mass balance process $W_{ijt} = \mu_{ij}W_{ij't} \quad i\in I,\ j\in J_i,\ j'\in JM_i, t\in T$

Capacity $W_{ijt} \le Q_{it} \quad i\in I,\ j\in JM_i, t\in T$

Mass balance chemicals $V_{j,t-1} + \sum_{i\in O_j} W_{ijt} + P_{jt} = V_{jt} + \sum_{i\in I_j} W_{ijt} + S_{jt} \quad j\in J, t\in T$

Shortfalls $SF_{jt} \ge d^U_{jt} - S_{jt} \quad j\in J, t\in T$

Purchases $a^L_{jt} \le P_{jt} \le a^U_{jt}$

Sales $d^L_{jt} \le S_{jt} \le d^U_{jt}$

$j\in J, t\in T$ (applies to Purchases and Sales)

Limit inventory $V_{jt} \le V^U_{jt} \quad j\in J, t\in T$

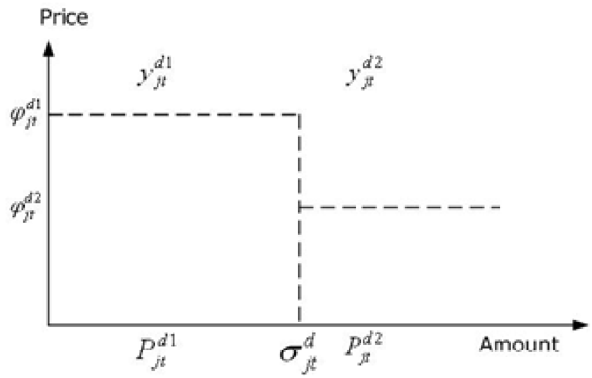
$$0 \le SF_{jt} \le SF^U_{jt} \quad j\in J, t\in T$$

$$S_{jt}, P_{jt}, W_{it}, V_{jt} \ge 0$$

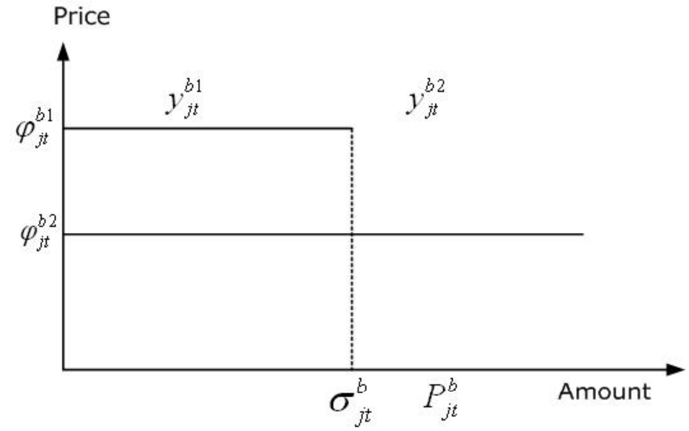
What if prices not fixed but given by contracts?

Modeling of Contracts with MILP

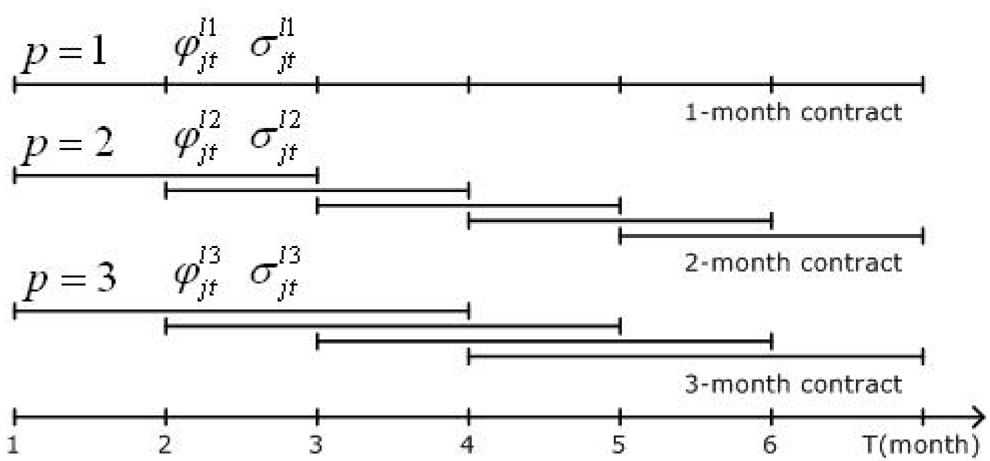
. Discount after σ_{jt}^{d} amount.



Bulk discount



Fixed-duration contracts



Disjunctive constraints => **MILP constraints (hull relaxation)**

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Computational Results

38 processes, 25 chemicals 10 time periods

	Case	0-1 variables	Cont. variables	Constraints	CPU time [s]	Time periods	Solution [10^5 $]
Fixed prices	1	0	12,606	13,416	0.18	10	18,085.95
Contracts	2	6,160	40,606	46,002	0.95	10	22,073.06

ILOG CPLEX Dec 1, 2008 22.9.2 LNX 7311.8080 LX3 x86/Linux
Cplex 11.2.0, GAMS Link 34

MIP Presolve eliminated 44425 rows and 38571 columns.
Reduced MIP has 909 rows, 1367 columns, and 3267 nonzeros.
Reduced MIP has 270 binaries, 0 generals, 0 SOSs, and 0 indicators.

Implied bound cuts applied: 3
Flow cuts applied: 40
Gomory fractional cuts applied: 15
MIP Solution: 22073.060039 (959 iterations, 21 nodes)

Synergy between CPLEX (presolve) and GDP (tight bounds)!

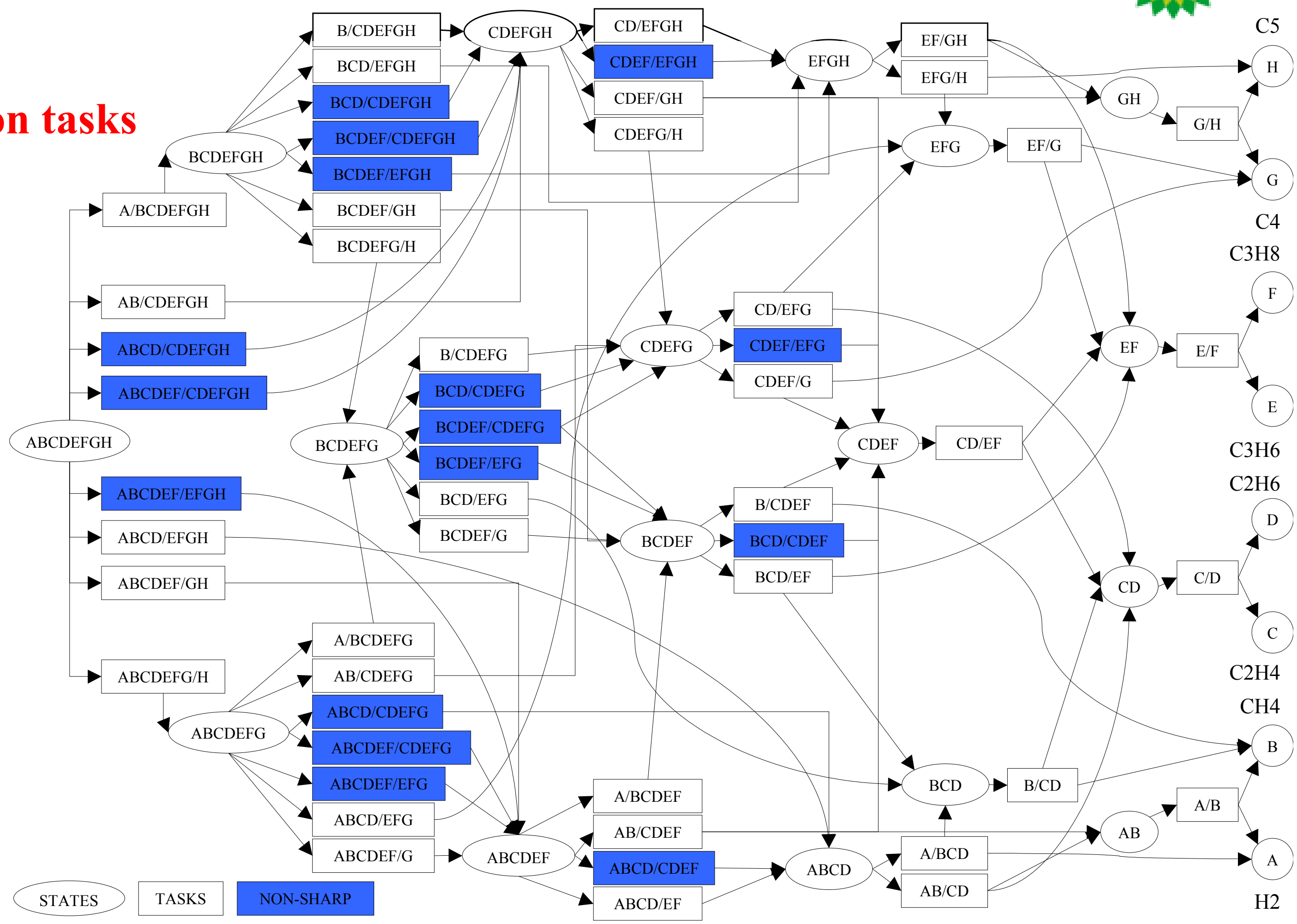
Superstructure Separations Olefins Plant

(Lee, Foral, Logsdon, Grossmann, 2003)

25 states
53 separation tasks

A- H_2
B- CH_4
C- C_2H_4
D- C_2H_6
E- C_3H_6
F- C_3H_8
G- C_4
H- C_5

Feed



GDP→big-M MINLP: 5,800 0-1 vars, 24,500 cont. vars., 52,700 constraints ~3hrs CPU-time

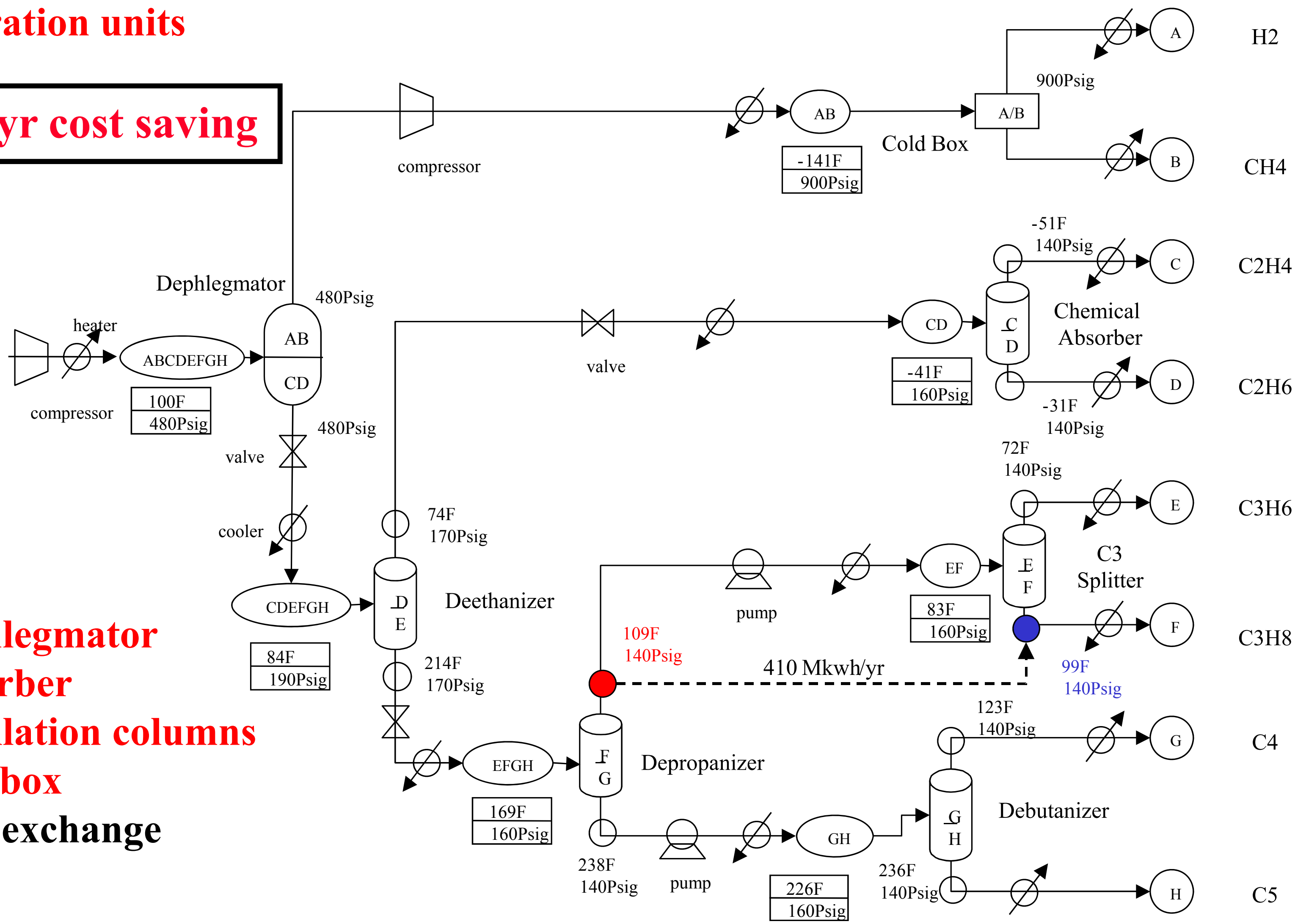
MINLP optimal solution

Dephlegmator first process

7 separation units

Total cost: 110.82 MM$/yr

20M$/yr cost saving



1 dephlegmator
1 absorber
4 distillation columns
1 cold box
1 heat exchange

Global Optimization Algorithms

Algorithms based on spatial branch and bound method and use of underestimators/convex envelopes *(Horst & Tuy, 1996)*

•Nonconvex NLP/MINLP

- **αBB** — *(Adjiman, Androulakis & Floudas, 1997; 2000)*
- **BARON (Branch and Reduce)** — *(Ryoo & Sahinidis, 1995, Tawarmalani and Sahinidis, 2002)*
- **Branch and cut** — *(Kesavan, Allgor, Gatzke and Barton, 2004)*
- **Branch and Contract** — *(Zamora & Grossmann, 1999)*
- **Transformation signomials** — *(Bjoerk, Lindberg, Westerlund, 2002)*
- **Couenne (COIN-OR)** — *(Belotti & Margot, 2008)*

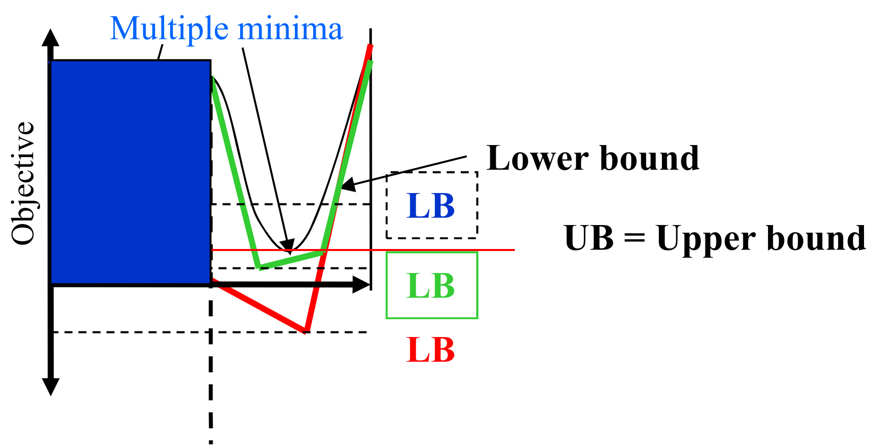
•Nonconvex GDP

- **Two-level Branch and Bound** — *(Lee & Grossmann, 2001)*
- **Bound strengthening** — *(Ruiz, Grossmann, 2010)*

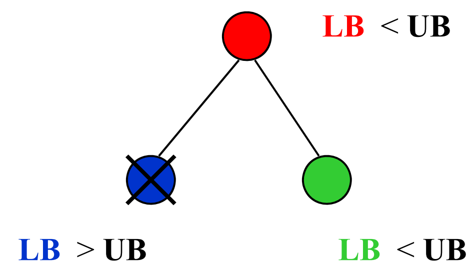
Spatial Branch and Bound to obtain the Global Optimum

- Guaranteed to converge to global optimum given a certain tolerance between lower and upper bounds

Global optimum search



Branch and bound tree



Progress BARON 1998-2006

Sahinidis (2008)

26 problems from *globallib* and *minlplib*

	Minimum	Maximum	Average
Constraints	2	513	76
Variables	4	1030	115
Discrete variables	0	432	63

Impact of Algorithmic Improvements

	BARON 1998	BARON 2006
# Nodes	23,031,434	253,754
CPU sec	275,163	20,430

 # Nodes reduction factor 100 !   CPU-time reduction factor > 10!

Large scale water network problem

4 feeds, 6 process units, 4 treatment units, 3 contaminants *Ahmetovic, Grossmann (2011)*

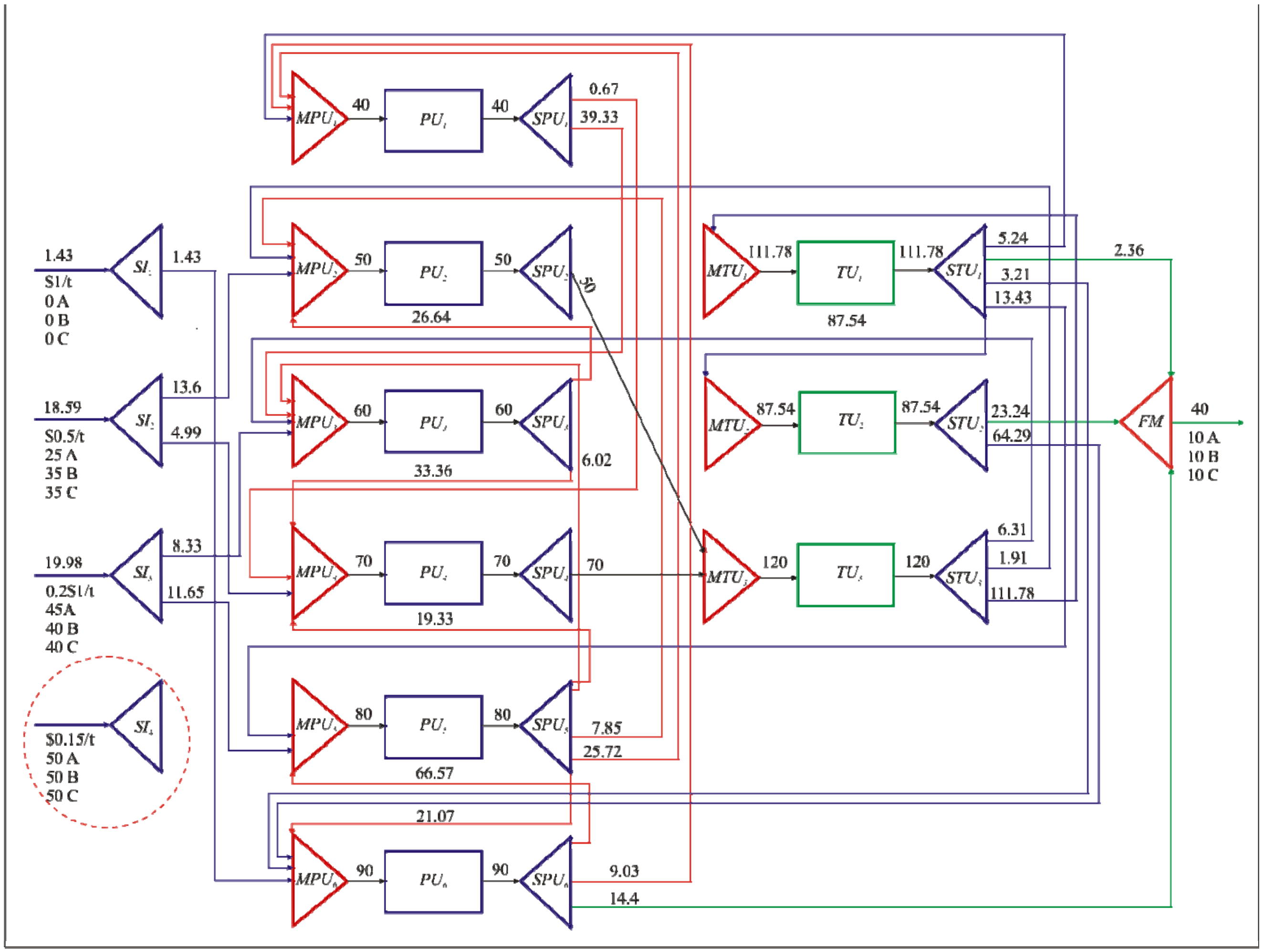
Optimal Freshwater Consumption

40 t/h

vs

390 t/h

conventional



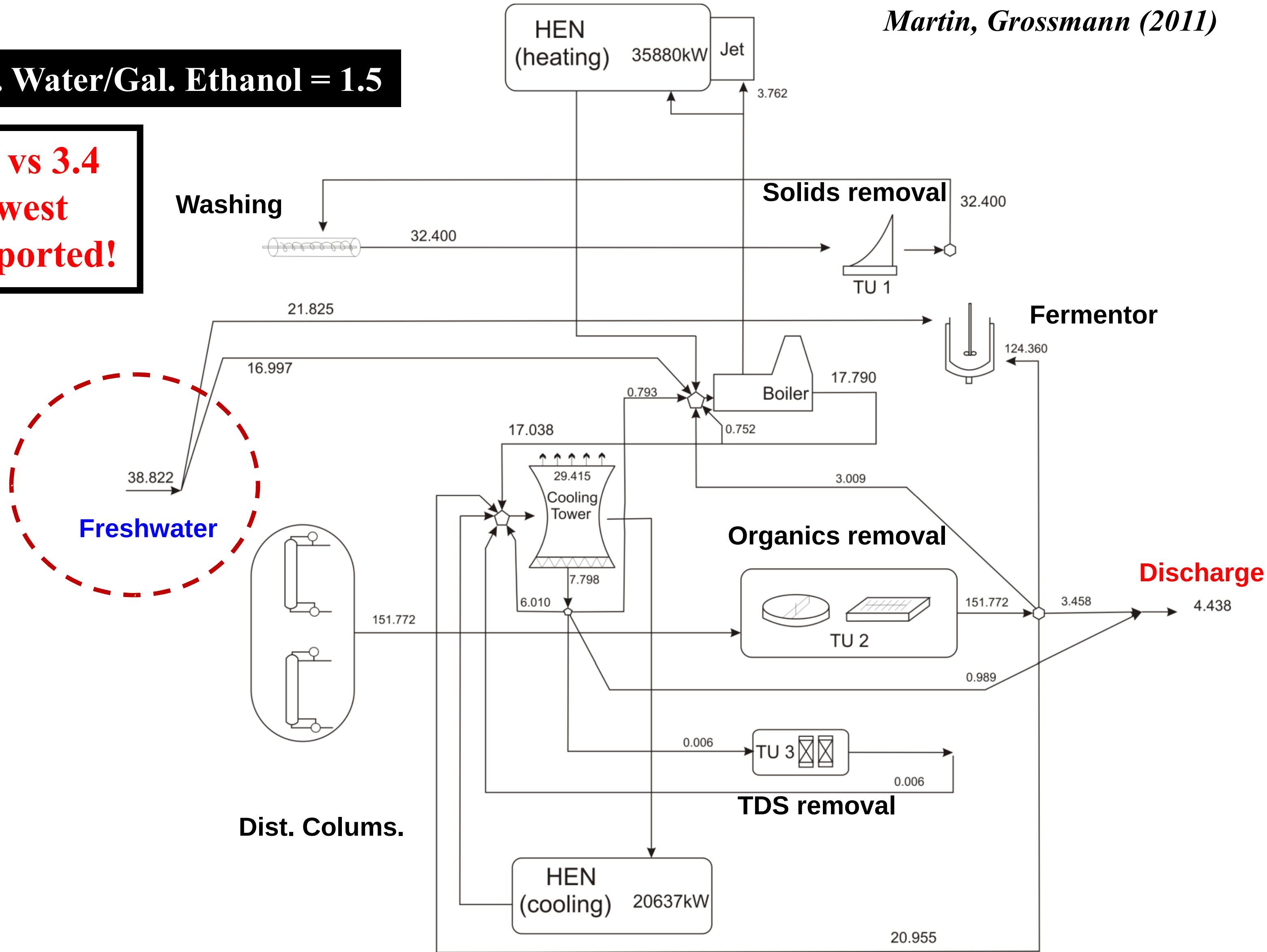
NLP: 232 variables, 121 constraints BARON: 2 secs

Optimal Water Network: Corn Ethanol

Gal. Water/Gal. Ethanol = 1.5

1.5 vs 3.4 Lowest Reported!

Martin, Grossmann (2011)



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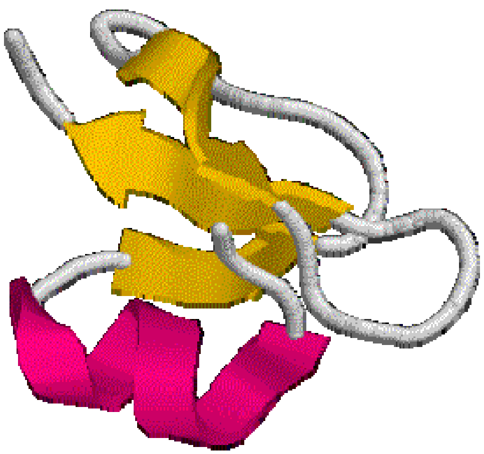
-Ahmetović , E., Martin, M. Grossmann, (2009) I&ECR. **2010, *49, 7972–7982***

De Novo Protein Design *(Floudas)*

<u>Define target template</u>

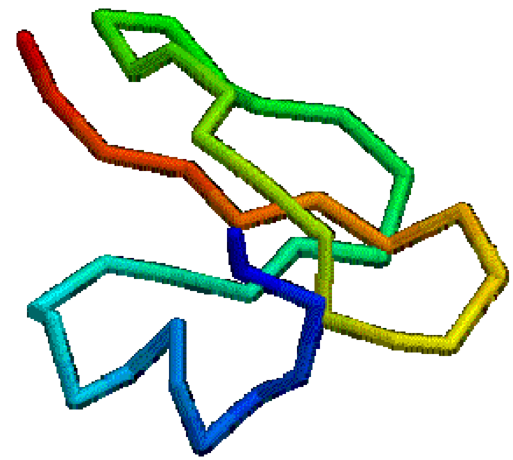
Backbone coordinates for N,Ca,C,O
and possibly Ca-Cb vectors from PDB



Human b-Defensin-2
hbd-2 (PDB: 1fqq)

<u>Design folded protein</u>

Which amino acid sequences will
stabilize this target structure ?



Full sequence design

In silico sequence selection => MILP

Fold specificity => Global optimization

=> New improved inhibitors ***(Klapeis, Floudas, Lambris, Morikis, 2004)***

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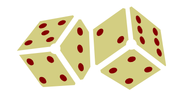
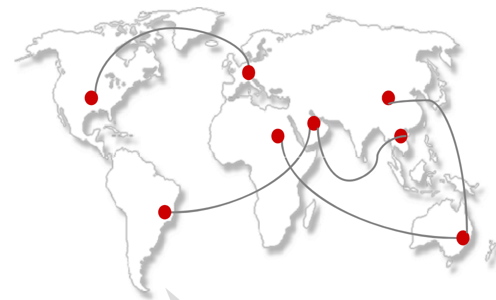


Risk Management

Global Sourcing Project with Uncertainties

You, Wassick, Grossmann (2009)



~ 100 facilities
~ 1,000 customers
~ 25,000 shipping links/modes

- Given
  - Minimum and initial inventory
  - Inventory holding cost and throughput cost
  - Single sourcing and minimum sourcing
  - Transport times of all the transport links
  - Uncertain production reliability and demands
- Determine
  - Inventory level, transportation and sale amounts

• Objective: Minimize Cost

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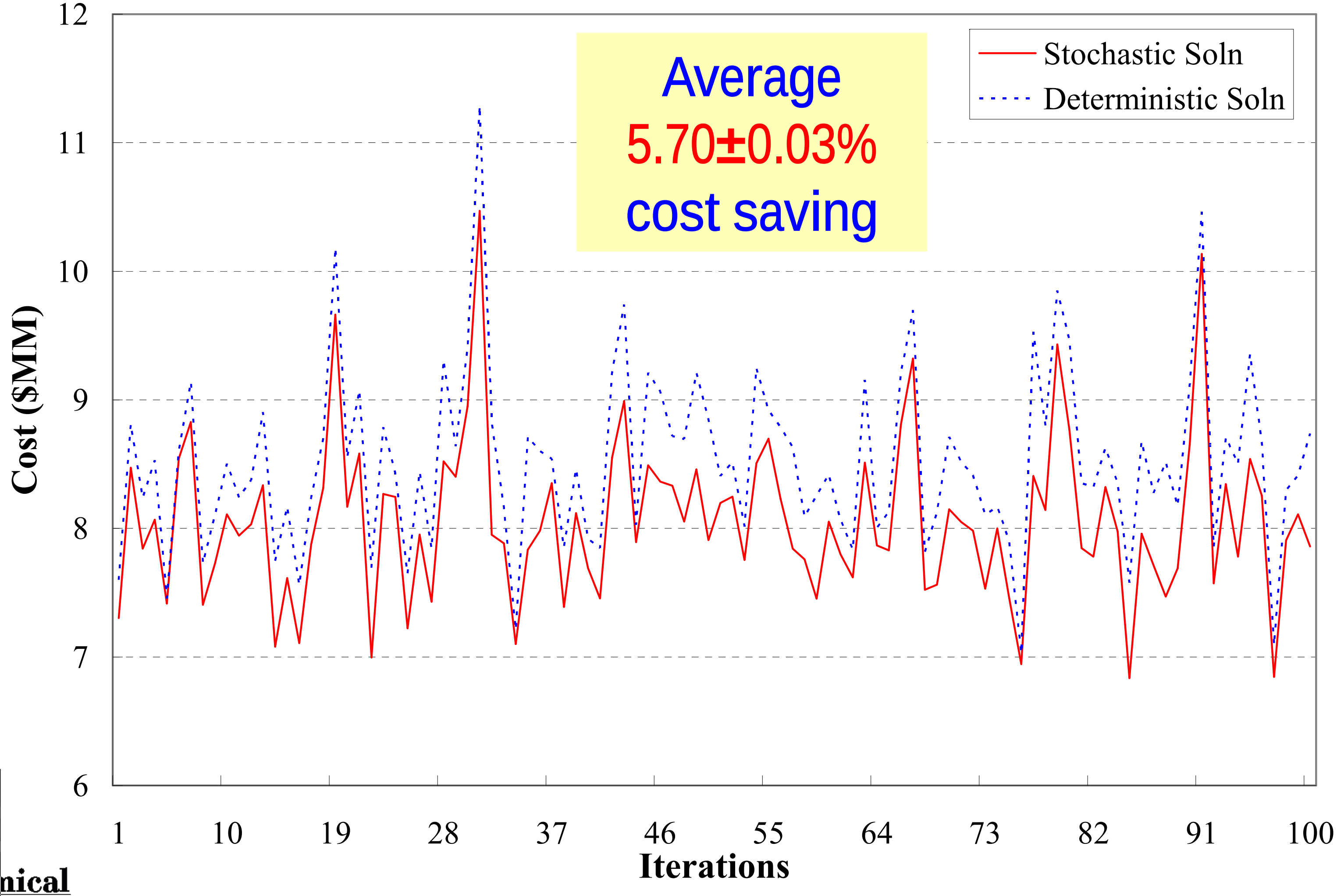
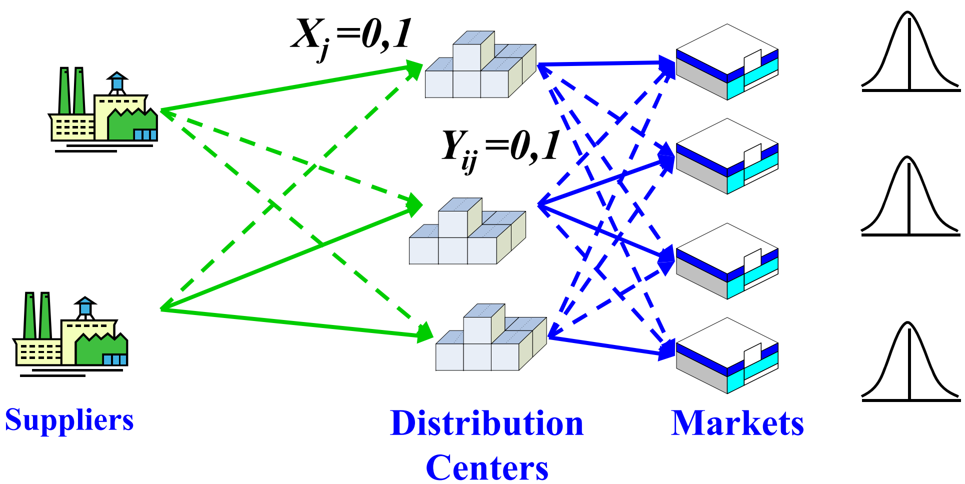
Simulation results to assess benefits stochastic model



Supply Chain Design with Single-Stage Stochastic Inventory

You, Grossmann (2009)

- **Given: A supply chain superstructure (single-product)**
  - **Including fixed suppliers, markets and potential DC locations**
  - **Each market has uncertain demand, only DCs hold inventory with (Q, r) policy**
  - **Assume all DCs have identical lead time L (lumped to one supplier)**



=> Nonconvex MINLP

Determine: Network: number of DCs and their locations, assignments between retailers and DCs (single sourcing), shipping amounts *⇒Linear*

Inventory: number of replenishments, order quantity, safety stock *⇒ Nonlinear*

150 DC, 150 markets: Lagrangean Relaxation: decomposition by Distribution Centers
MINLP: 150 0-1 var., 22,800 cont. var., 22,800 constr. 3061s CPU-time) ***(<1% gap)***

Conclusions

1. **Discrete/continuous optimization methods have had**

   - ***tremendous*** ***progress in MILP***
   - ***very significant progress in MINLP/GDP***
   - ***good progress in global MINLP/GDP***

2. **Theory has contributed to progress:**

   - ***sequential convexification for MILP***
   - ***concepts of disjunctive programming => MINLP and GDP***

   Complemented by algorithmic implementations/new computer architectures

3. **Many of models/algorithms used increasingly by industry**

Major remaining challenges:

- *Improvement of relaxations for MILP and MINLP*
- *Improvement of relaxations for global optimization*
- *Large-scale computations for nonconvex MINLP/GDP*
- *Effective algorithms for Mixed-Integer Dynamic Optimization*
- *Effective extension to stochastic programming, parametric programming*

Conclusions

1. **Enterprise-wide Optimization area of great industrial interest**
   Great economic impact for effectively managing complex supply chains and complex manufacturing facilities

2. **Two key components: Planning and Scheduling**
   Modeling challenge:
   Multi-scale modeling (temporal and spatial integration)

3. **Computational challenges lie in:**
   a) Large-scale optimization models (decomposition, advanced computing)
   b) Handling uncertainty (stochastic programming)

Scope for significant economic savings

Future challenges

1. Logic-based Optimization

Facilitate modeling

Exploit logic for more efficient solution

2. Global Optimization

Effectively solve nonconvex MINLP problems

3. Stochastic Mixed-integer Programming

Reduce computational times by order of magnitude

Generalized Disjunctive Programming (GDP) Model

$$\min Z = \sum_i \left(IC_i + CC_i + UC_i \right)$$ **Cost**

$$s.t. \quad Ax = 0$$ **Mass balances**

$$feq(P_i, T_i), \quad \forall i \in I$$ **Equilibrium Eqtns.**

Separation choice

$$\bigvee_{s \in S_i} \begin{bmatrix} YS_{i,s} \\ x_i^{top} = RT_i x_i^{feed} \\ x_i^{btm} = RB_i x_i^{feed} \\ \bigvee_{st \in ST_s} \begin{bmatrix} YT_{s,st} \\ mass\ balance: fm(x_i) = 0 \\ energy\ balance: fe(x_i, T_i, P_i, Q_i) = 0 \\ \cos t\ \ fuction: (IC_i, UC_i) = fc(x_i, T_i, P_i, Q_i) \end{bmatrix} \end{bmatrix}, \quad \forall i \in I$$

$$\begin{bmatrix} YZ_{i,k} \\ T_i^C \geq T_k^R + EMAT \\ QEX_{i,k} \geq 0 \\ (IC_i, UC_i) = fz(x_i, T_i, P_i, QEX_{i,k}) \end{bmatrix} \vee \begin{bmatrix} \neg YZ_{i,k} \\ QEX_{i,k} = 0 \end{bmatrix}, \quad \forall i \in I, \forall k \in K$$ **Heat exchange**

$$\begin{bmatrix} YC_i \\ (T_i, P_i)_{out} = fp_1(T_i, P_i)_{in} \\ CR_L \leq P_i^{out} / P_i^{in} \leq CR_U \\ CC_i = fp_2(x_i, T_i, P_i) \end{bmatrix} \vee \begin{bmatrix} \neg YC_i \\ (T_i, P_i)_{out} = (T_i, P_i)_{in} \\ CC_i = 0 \end{bmatrix}, \quad \forall i \in I$$ **Compression**

Can we obtain stronger relaxations?

Regular Form (RF): Form represented by the intersection of the unions of convex sets.

$$F = \bigcap_{t \in T} S_t \quad \text{where } S_t = \bigcup_{i \in Q} P_i \quad t \in T \quad \text{and} \quad P_i \text{ is a convex set}$$

Basic Step: Intersect a pair of disjunctions & bring into DNF

for some $r, s \in T$ $\quad S_r \cap S_s = S_{rs} = \bigcup_{\substack{i \in Q_r \\ t \in Q_s}} (P_i \cap P_t)$

Example: $F = S_1 \cap S_2 \qquad S_1 = (P_{11} \cup P_{21}) \qquad S_2 = (P_{12} \cup P_{22})$

Apply Basic Step to:

$$S_1 \cap S_2 = (P_{11} \cup P_{21}) \cap (P_{12} \cup P_{22})$$

=> $$S_{12} = (P_{11} \cap P_{12}) \cup (P_{11} \cap P_{22}) \cup (P_{21} \cap P_{12}) \cup (P_{21} \cap P_{22})$$

Balas (1974, 1979, 1985) addressed linear disjunctive programs

Hierarchy of relaxations for nonlinear convex GDP

Theorem 2: For $i = 0,1, 2\ldots. t$ let $F_i = \bigcap_{j \in T_i} S_j$ be a sequence of regular forms of a disjunctive set such that F_i is obtained from F_{i-1} by the application of a basic step, then:

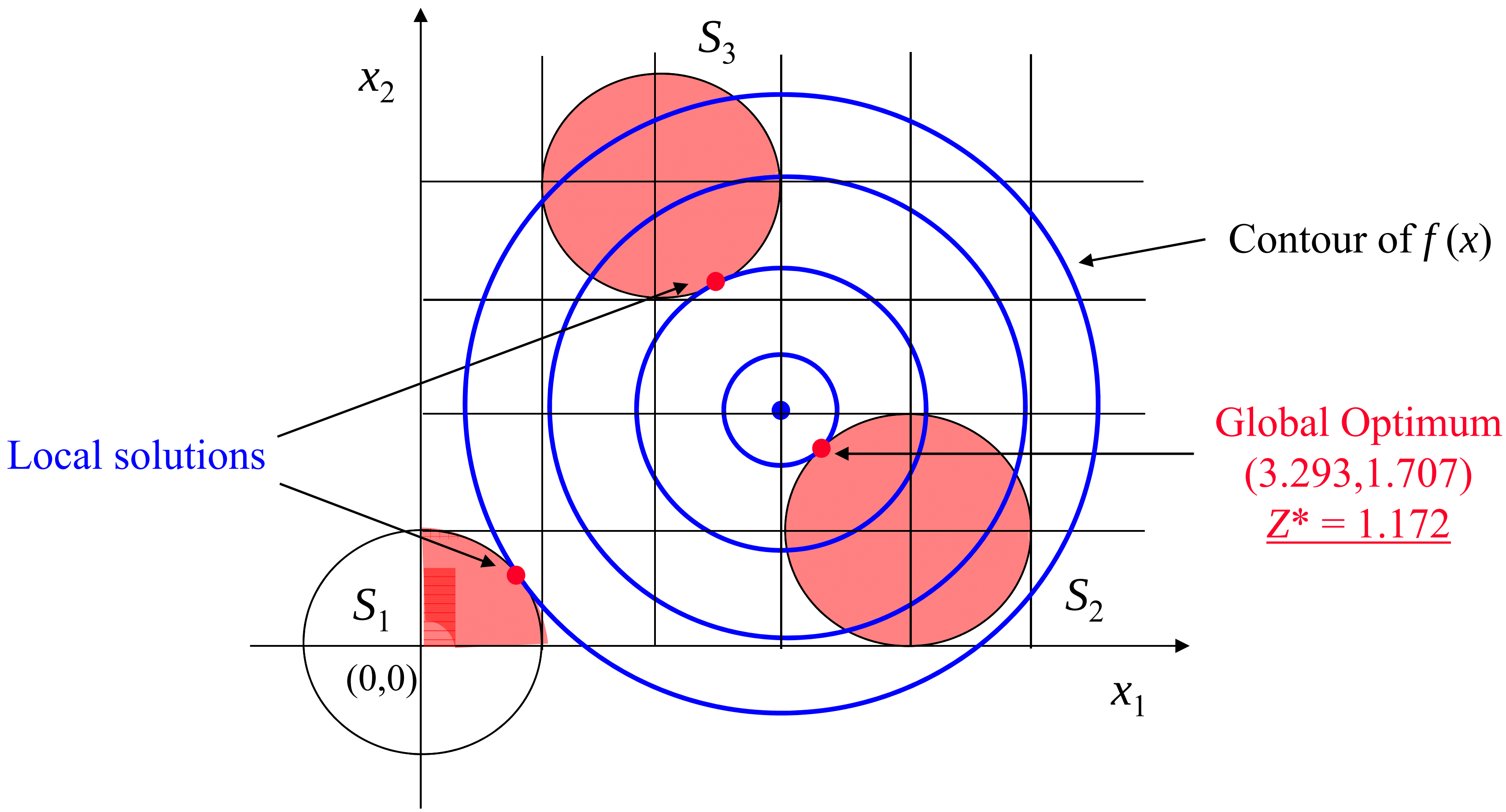
$$h-rel(F_i) \subseteq h-rel(F_{i-1})$$

Tighter region!

GDP Example

- **Find $x \geq 0$, $(x \in S_1) \vee (x \in S_2) \vee (x \in S_3)$**

  to minimize $Z = (x_1 - 3)^2 + (x_2 - 2)^2 + c$



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Hull Relaxation (one basic step)

Apply basic step: Intersect inequality objective with disjunction

$$\min\ Z$$
$$s.t.$$

$$\begin{bmatrix} Y_1 \\ x_1^{\,2} + x_2^{\,2} \le 1 \\ c = 2 \\ Z \ge (x_1 - 3)^2 + (x_2 - 2)^2 + c \end{bmatrix} \vee \begin{bmatrix} Y_2 \\ (x_1 - 4)^2 + (x_2 - 1)^2 \le 1 \\ c = 1 \\ Z \ge (x_1 - 3)^2 + (x_2 - 2)^2 + c \end{bmatrix} \vee \begin{bmatrix} Y_1 \\ (x_1 - 2)^2 + (x_2 - 4)^2 \le 1 \\ c = 2 \\ Z \ge (x_1 - 3)^2 + (x_2 - 2)^2 + c \end{bmatrix}$$

$$Y_1 \underline{\vee} Y_2 \underline{\vee} Y_3 = True$$

Relaxation of convex hull MINLP reformulations yields optimal solution!

$$Z^{rel} = 1.172$$

Solves as an NLP!

GDP Model (continued)

Logic Propositions

$$\vee YS_{i,s} \qquad \forall i \in I$$

$$YS_{i,s} \Rightarrow \vee YT_{s,st} \qquad \forall st \in ST_s, \forall s \in S_i, \forall i \in I$$

$$\neg YS_{s,st} \Rightarrow \neg YZ_{i,k} \qquad \forall st \in ST_s, \forall s \in S_i, \forall i \in I, \forall k \in K$$

Variable Bounds

$$0 \le x_i \le x^{UP}; T^{LO} \le T_i \le T^{UP}; P^{LO} \le P_i \le P^{UP}, \quad \forall i$$

$$0 \le RT_i, RB_i \le 1 \qquad \forall i$$

$$0 \le IC_i, CC_i, UC_i \qquad \forall i$$

$$YS_{i,s}, YT_{s,st}, YZ_{i,k}, YC_i \in \{true, false\} \quad \forall i, s, st, k$$

$$0 \le Q_i, QEX_{i,k} \quad \forall i, k$$

$$T^{LO} \le T_i^C, T_k^R \le T^{UP} \quad \forall i, k$$

MINLP Model

- **GDP reformulated as a MINLP**

- **Problem Size**
  - **No. of 0-1 variables = 5,800**
  - **No. of variables = 24,500**
  - **No. of constraints = 52,700**

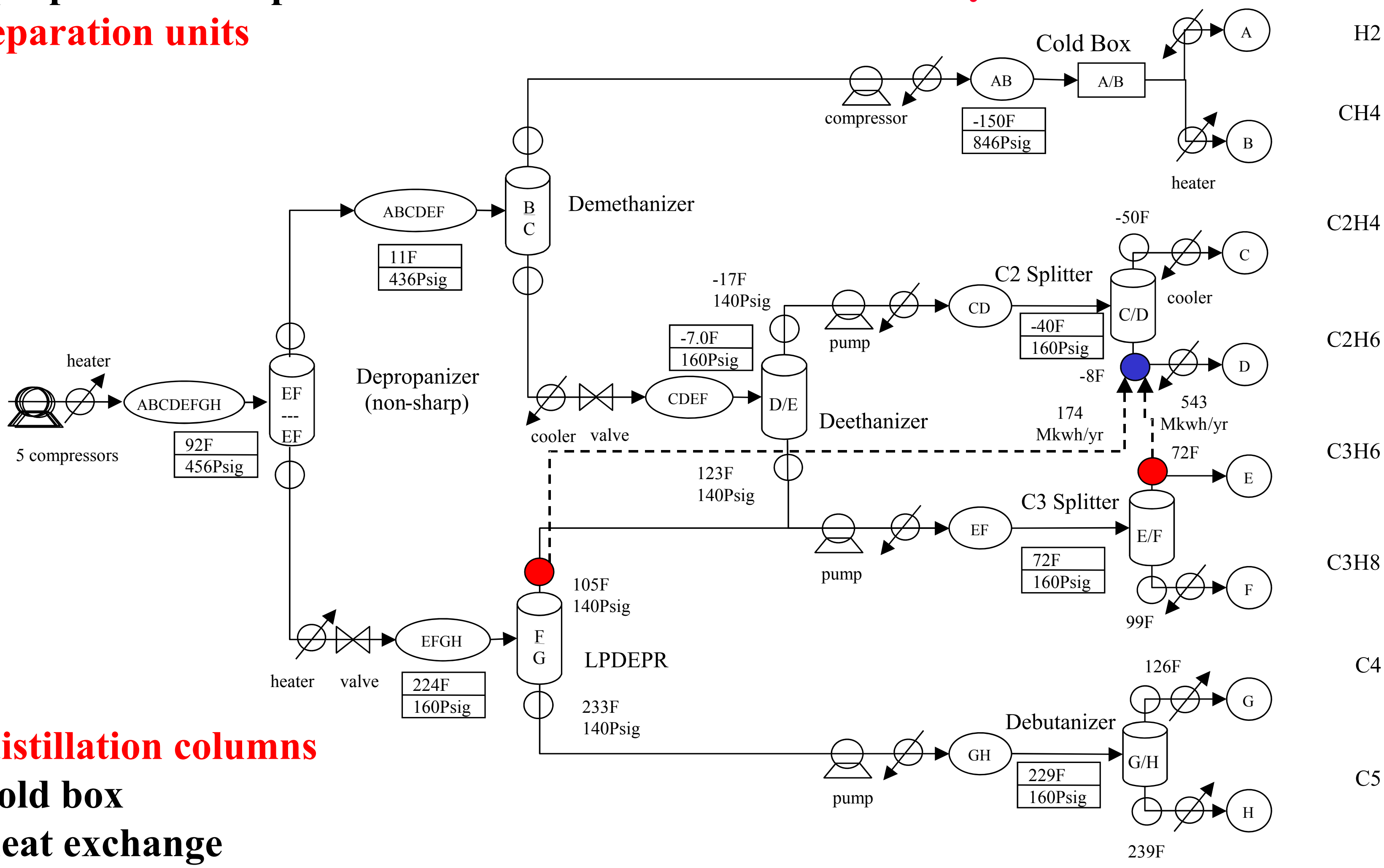
- **GAMS/DICOPT**
  - **NLP solver: CONOPT2/ MIP solver: CPLEX**
  - **CPU time ~ 3 hrs on Pentium III PC**

Optimized base case design

Depropanizer first process

8 separation units

Total cost: 131.74MM$/yr



7 distillation columns

1 cold box

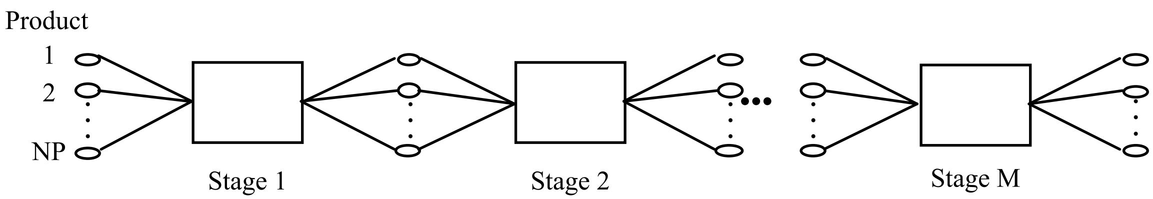
2 heat exchange

Continuous multistage plants

Pinto, Grossmann (1996)

Cyclic schedules *(constant demand rates, infinite horizon)*

Intermediate storage



Given :

N Products
Transition times *(sequence dependent)*
Demand rates

Determine :

PLANNING

Amount of products to be produced
Inventory levels

SCHEDULING

Cyclic production schedule
Sequencing
Lengths of production
Cycle time

Objective :

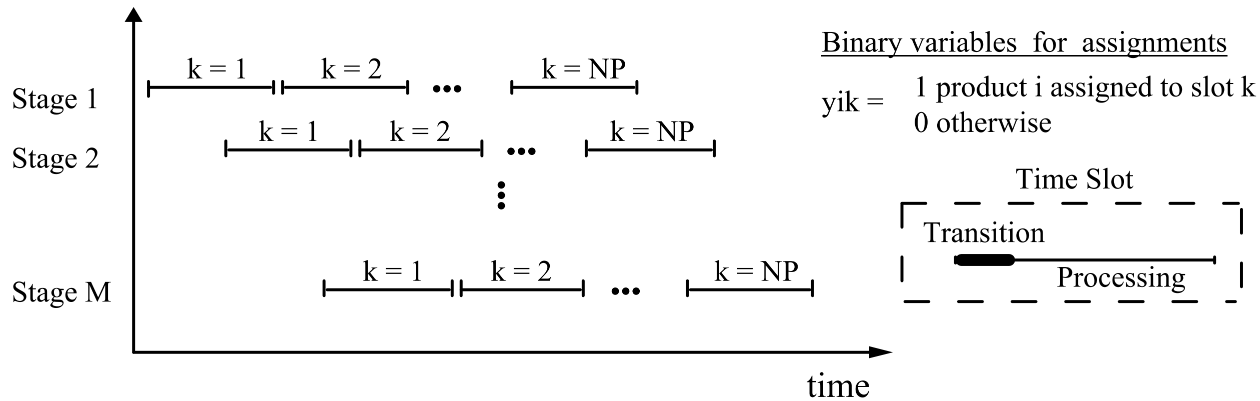
Maximize Profit = + Sales of products - inventory costs - transition costs

MINLP Model

Basic ideas :

a. NP products

b. NP time slots at each stage



a) Assignments of products to slots

b) Definition of transition variables

c) Processing rates, mass balances and amounts produced

d) Timing constraints

e) Inventory levels for intermediates

f) Demand constraints

=> Linear Constraints

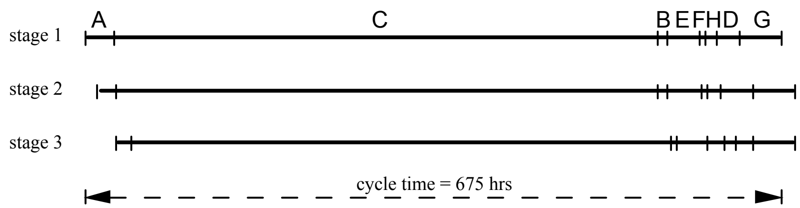
Objective function : Maximize Profit (Nonlinear)

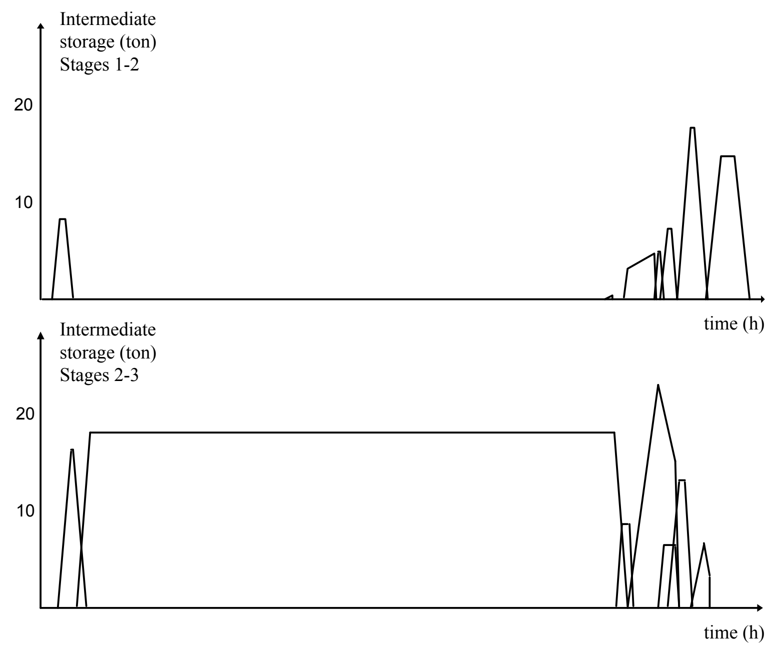
Example 3 stages, 8 products

MINLP model 448 binary 0-1 variables, 2050 continuous variables, 3010 constraints

DICOPT (CONOPT/CPLEX): 38.2 secs

Optimal solution Profit = $6609/h - 47% improvement

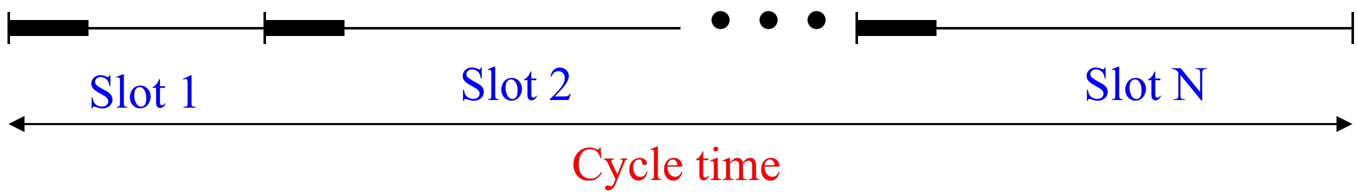


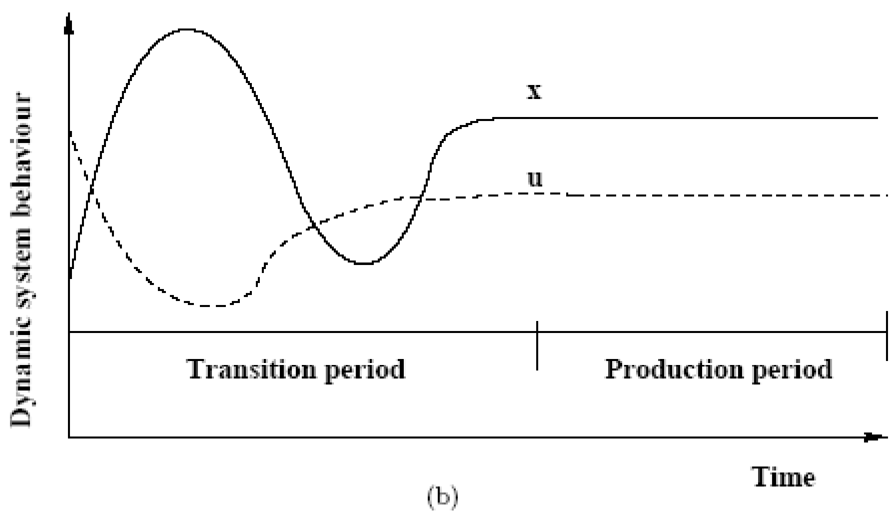


Simultaneous Cyclic Scheduling and Control of a Multiproduct CSTR Reactor

(MIDO) Mixed-integer Dynamic Optimization Problem ***Flores, Grossmann (2008)***

$$y_{il} = \begin{cases} 1 & product\ i\ \ assigned\ \ slot\ \ l \\ 0 & otherwise \end{cases}$$





Requires determining transition times

Use orthogonal collocation for converting dynamic eqtns into algebraic eqtns.

Mixed-Integer Dynamic Optimization solved as MINLP *(DICOPT or SBB)*

Outline

1. **Historical Evolution of Mathematical Programming**

2. **Progress in Mixed-integer Linear Programming**
   Impact on batch scheduling

3. **Progress in Mixed-integer Nonlinear Programming**
   Impact on optimal process operations

4. **Future challenges**

Motivation MINLP in PSE

Math Programming Approach
to Process Synthesis

Sargent, Gaminibandara (1977)   Grossmann, Santibanez (1980)

1. **Develop a superstructure of alternative designs**

2. **Develop an MINLP model to
select topology and parameters of design**

3. **Solve MINLP to extract optimum
design embedded in superstructure**

Hull Relaxation Formulation

- **Consider Disjunction $k \in K$**

$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \leq 0 \\ c = \gamma_{jk} \end{bmatrix}$$

- **Theorem: Convex Hull of Disjunction k** *(Lee, Grossmann, 2000)*
  - **Disaggregated variables v^j**

$$\{(x,c) \mid x = \sum_{j \in J_k} v^{jk}, \quad c = \sum_{j \in J} \lambda_{jk} \gamma_{jk},$$

$$0 \leq v^{jk} \leq \lambda_{jk} U^{k}_{jk}, \; j \in J_k$$

=> Convex Constraints

$$\sum_{j \in J_k} \lambda_{jk} = 1, \quad 0 < \lambda_{jk} \leq 1,$$

$$\lambda_{jk} g_{jk}(v^{jk} / \lambda_{jk}) \leq 0, \; j \in J_k \}$$

  - **λ_j - weights for linear combination**

- Generalization of Balas (1979)
Stubbs and Mehrotra (1999)

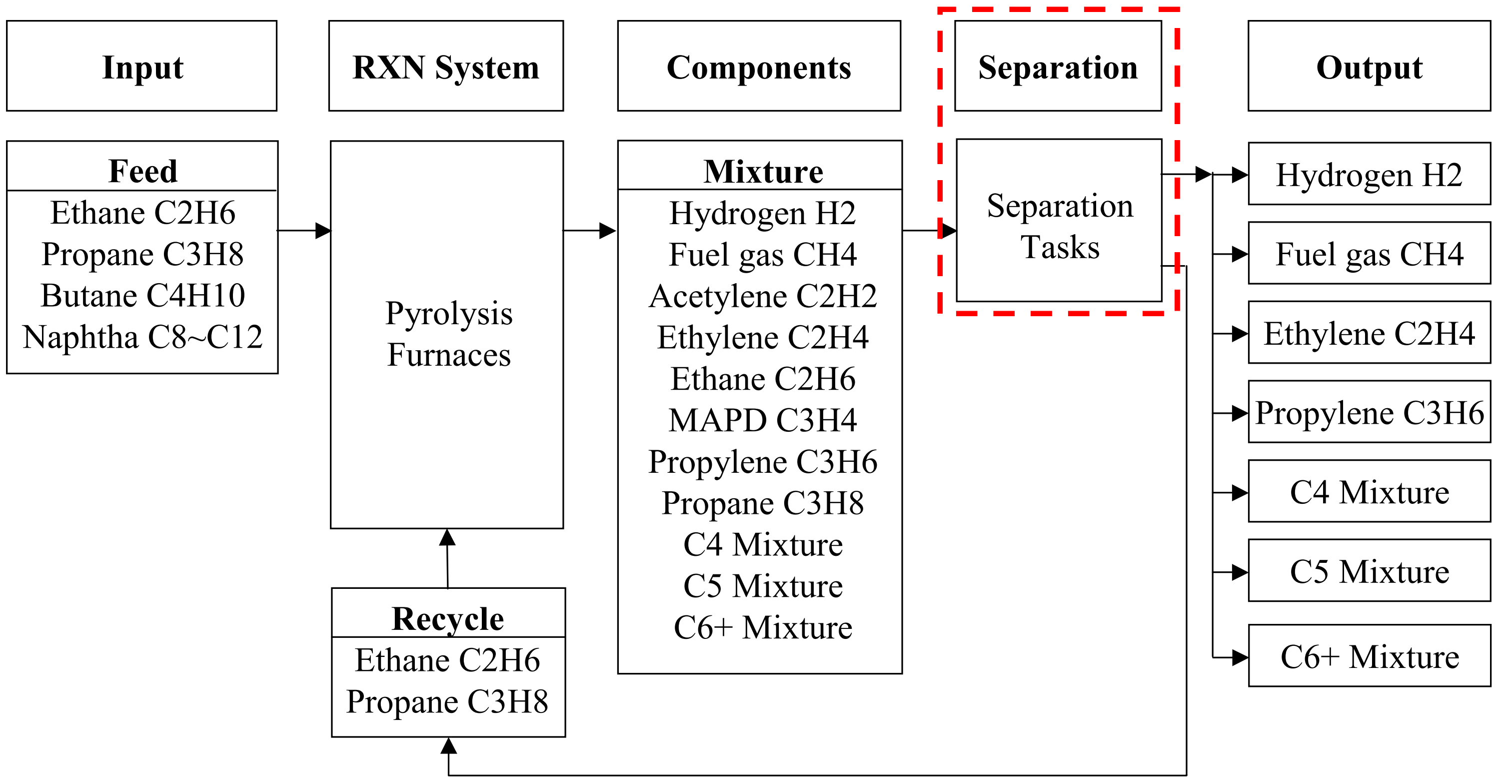
Hull relaxation: intersection of convex hull of each disjunction

Carnegie Mellon

Olefin Separation System *(BP)*

(Lee, Foral, Logsdon, Grossmann, 2003)

Goal: Synthesize optimal separation system



Alternative Separation Schemes

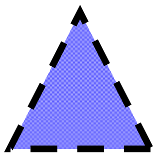
Separation Technologies

T1	Distillation column
T2	Physical absorption
T3	Membrane separator
T4	Dephlegmator
T5	Pressure swing adsorption (PSA)
T6	Cold box
T7	Chemical absorption

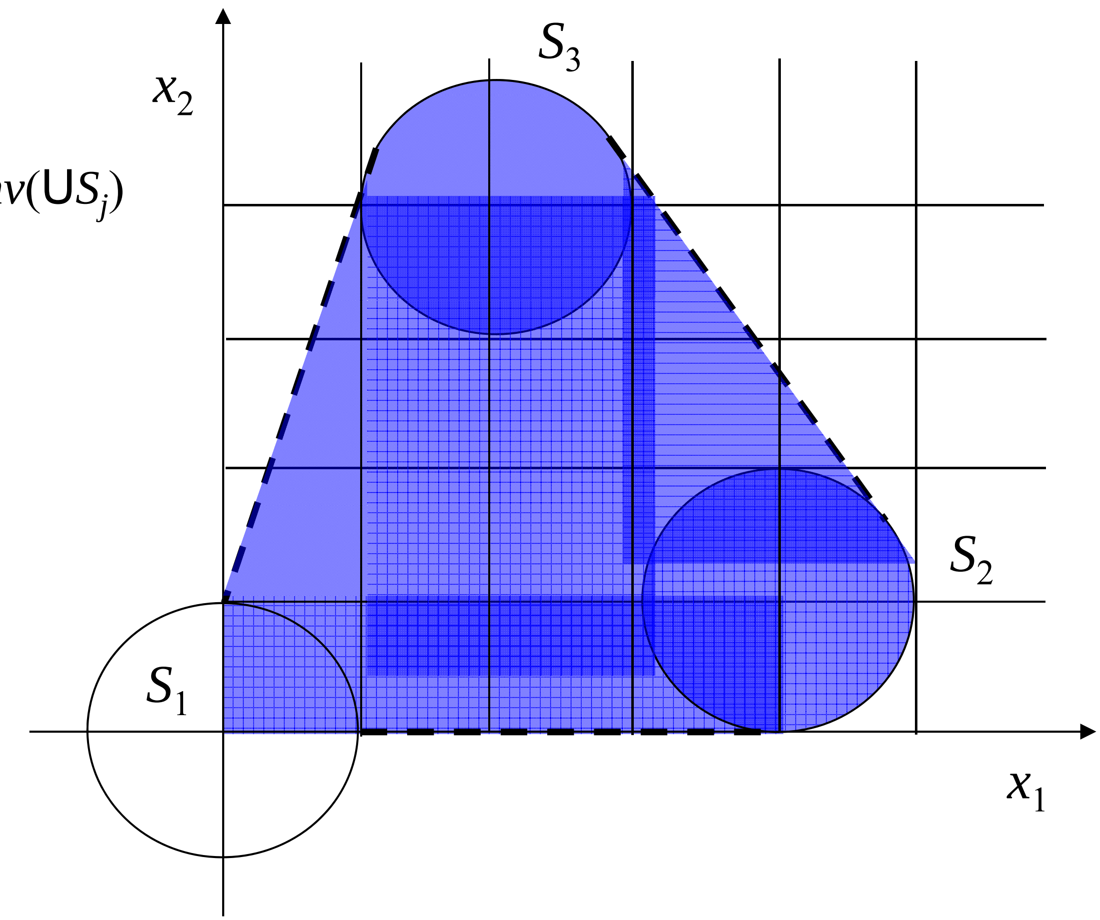
Feed Components

A	H_2	E	C_3H_6
B	CH_4	F	C_3H_8
C	C_2H_4	G	C_4
D	C_2H_6	H	C_5

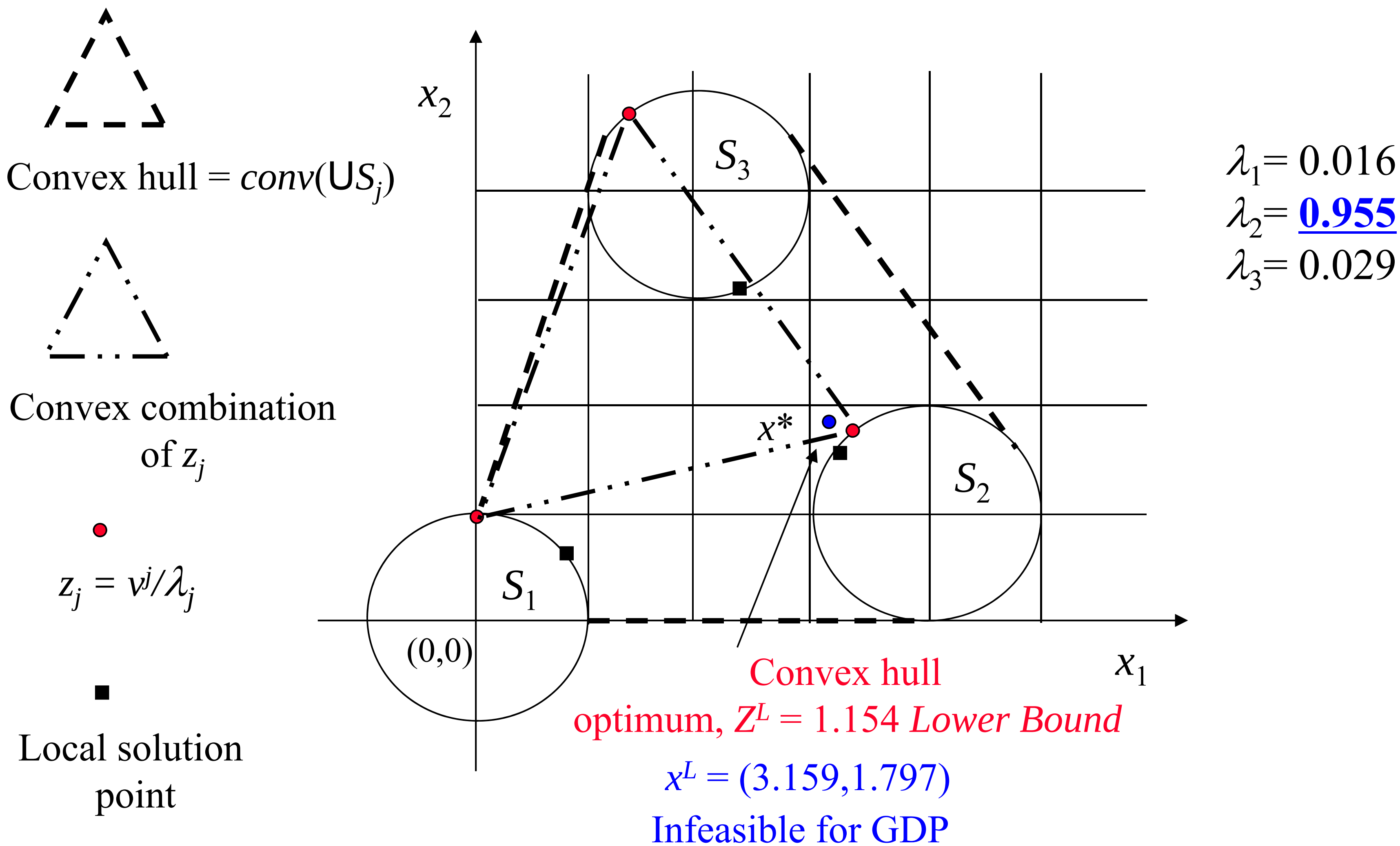
Example : convex hull



Convex hull = $conv(\cup S_j)$



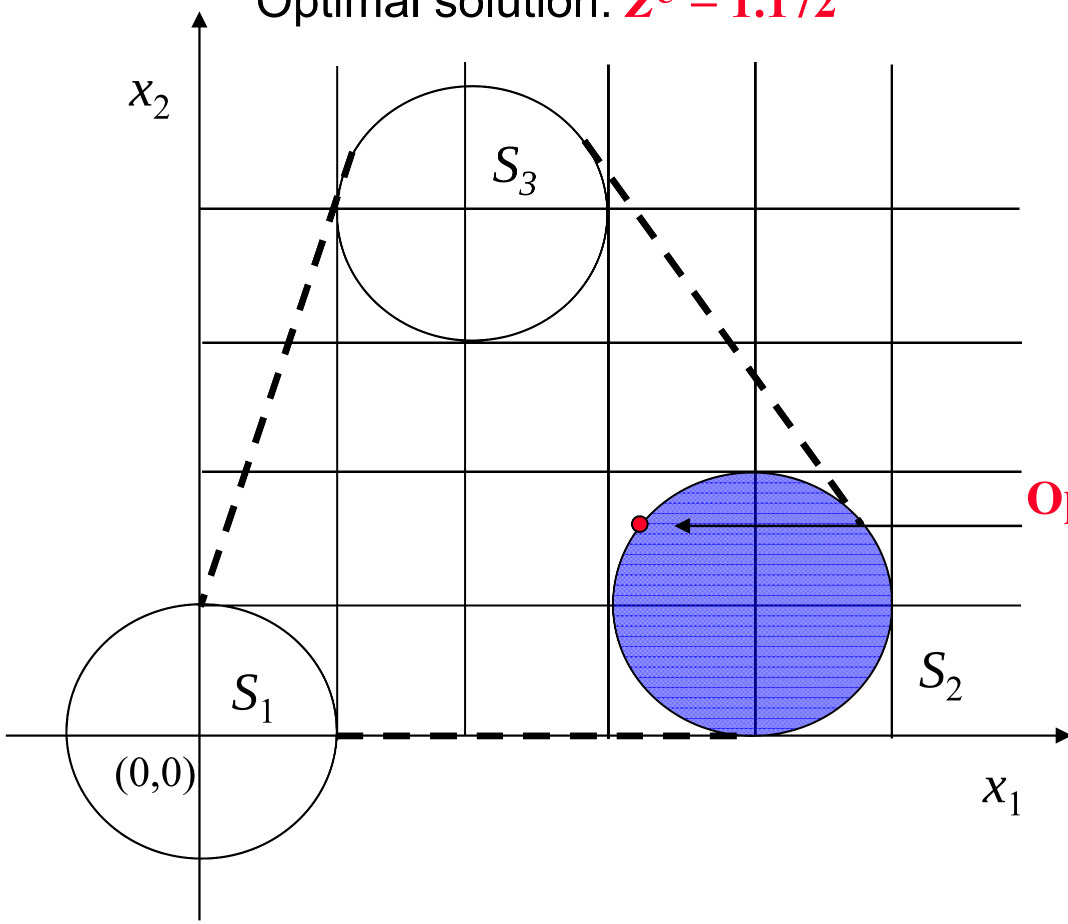
Example: CRP solution



Example : branch and bound

First Node: S_2

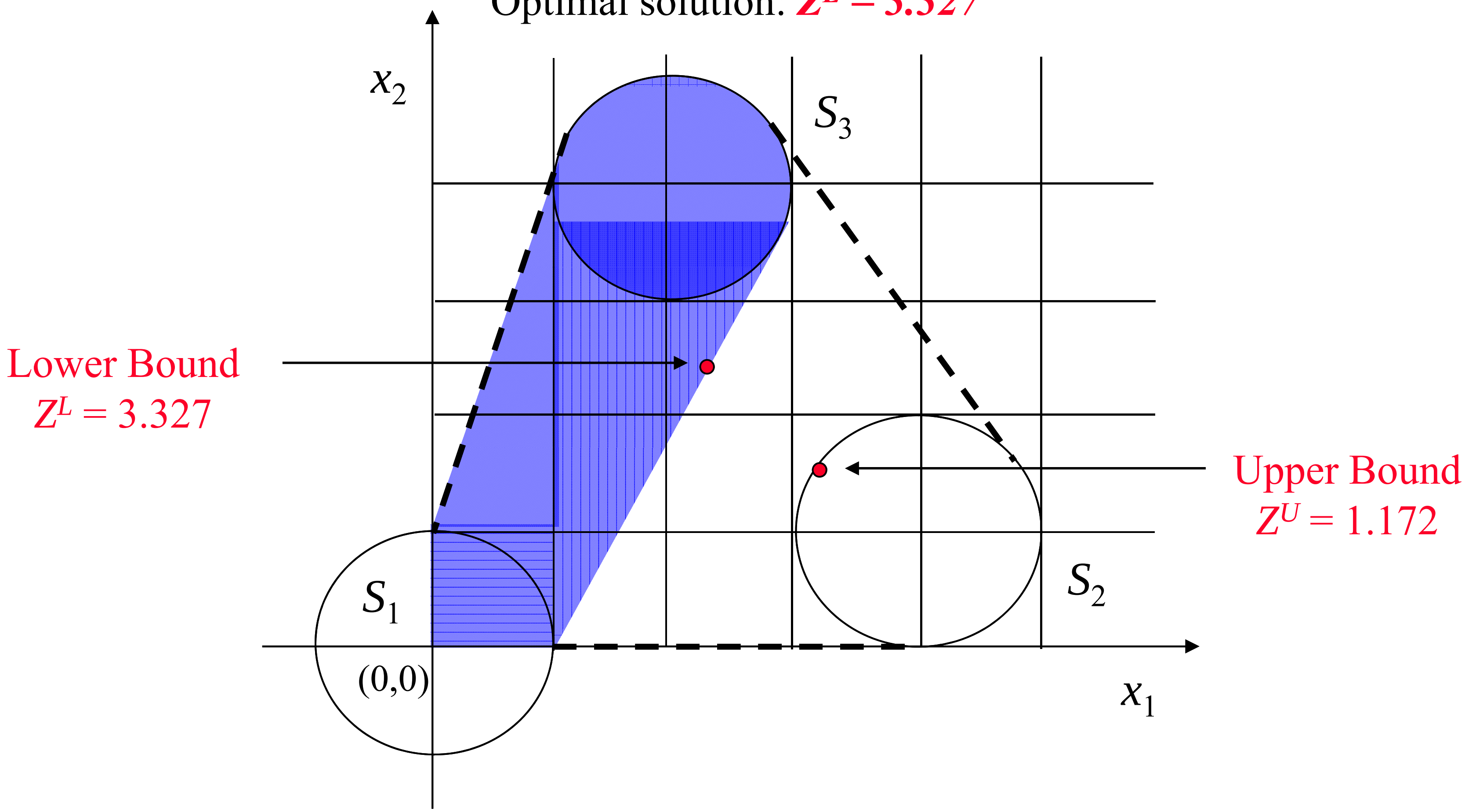
Optimal solution: $Z^U = 1.172$



Example : branch and bound

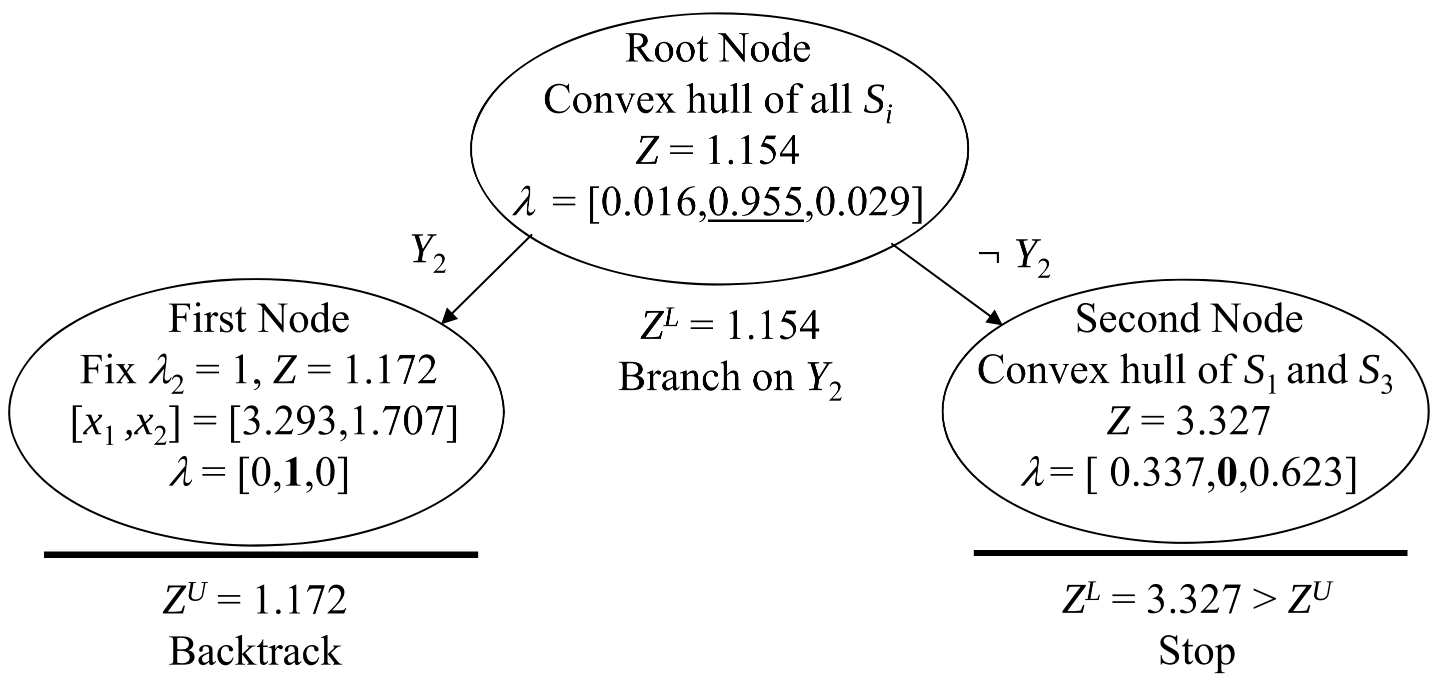
Second Node: ***conv(S_1 U S_3)***

Optimal solution: $Z^L = 3.327$



Example: Search Tree

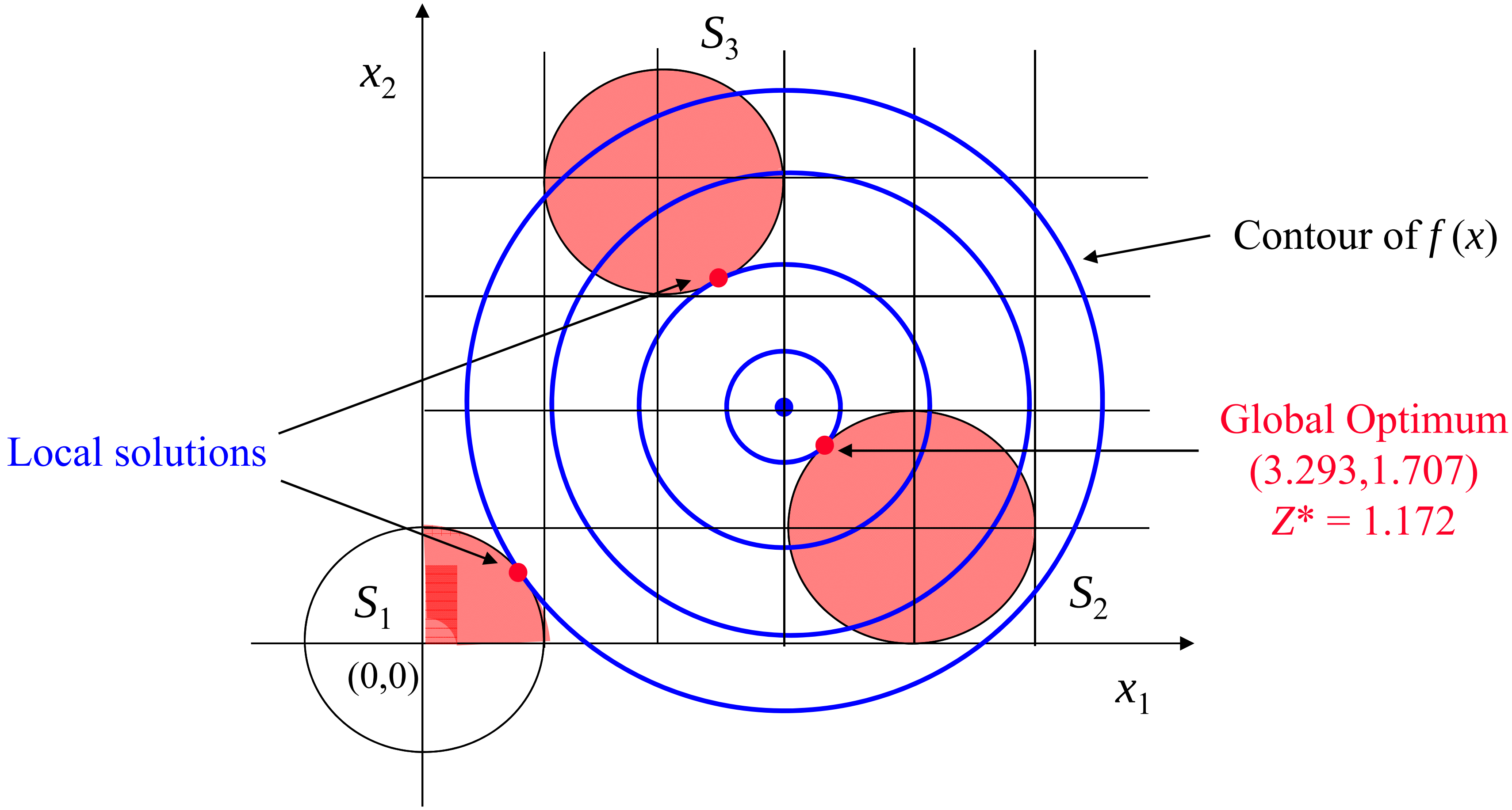
- **Branching Rule:** λ_j - the "weight" of disjunction
  - Fix Y_j as true: fix λ_j as 1.



GDP Example Revisited

- **Find x ≥ 0, $(x \in S_1) \vee (x \in S_2) \vee (x \in S_3)$ to minimize Z**

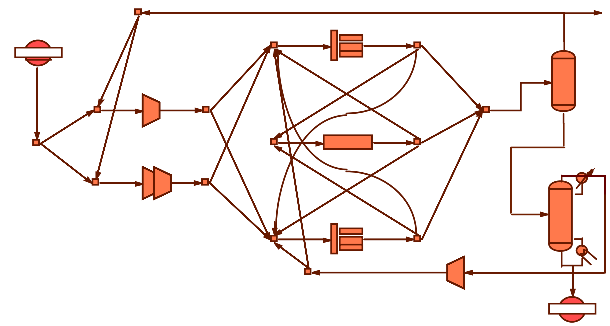
  Transfer objective as inequality $Z \geq (x_1 - 3)^2 + (x_2 - 2)^2 + c$



Applications of Mathematical Programming in Chemical Engineering

Process Design

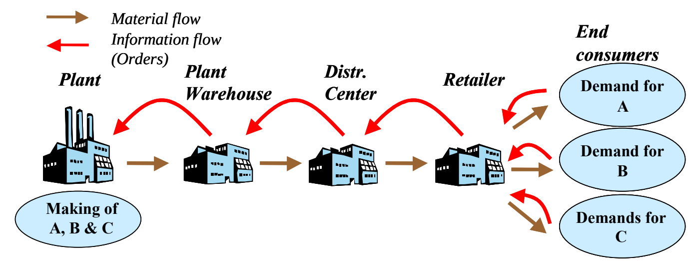
Process Synthesis



Production Planning

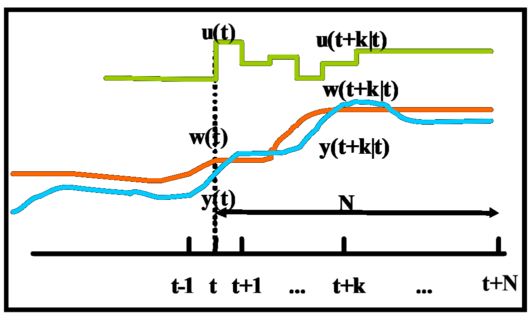
Process Scheduling

Supply Chain Management



Process Control

Parameter Estimation



Models: LP, MILP, NLP, MINLP

new problem representations and models

Progress in Linear Programming

Increases in computational speed 1987-2002

Bixby-ILOG (2002)

For 50,000 row LP model

Algorithms

Primal simplex in 1987 *(XMP) versus*

Best (primal,dual,barrier) 2002 ***(CPLEX 7.1)*** **2400x**

Machines

Sun 3/150

Pentium 4, 1.7GHz **800x**

Net increase: Algorithm * Machine ~ 1 900 000x

Two million-fold increase in speed!!

Proposed framework to obtain stronger relaxations for nonconvex GDP

(Bilinear and Concave GDP)

Ruiz, Grossmann (2009)

Basic idea:
Based on **relaxation of the nonconvex GDP as a linear GDP exploit** the **theory behind DP** to obtain **stronger relaxations**.

The **framework** consists of **two main phases**:

1- Generate a **valid <u>Linear</u> Generalized Disjunctive Program** *relaxation for the nonconvex GDP problem* (e.g. convex envelopes bilinear and concave).

2- Strengthen the *continuous relaxation of the* ***linear GDP*** obtained in phase 1 by **applying a set of basic steps**

The **hierarchy of relaxations** obtained by the application of basic steps is **valid for the original nonconvex GDP** problem

Big-M and HR vs. Proposed strengthening

All problems were solved using NLP branch-and-bound SBB/CONOPT 3.14 (GAMS)

Table: Performance using different reformulation strategies

		BM Approach			HR Approach			Proposed Approach		
Example	Opt.	LB	Nds	T(s)	LB	Nds	T(s)	LB	Nds	T(s)
Circles2D3	1.17	0.00	4	1.0	1.15	4	1.04	1.17	0	0.7
Circles2D36	2.25	0.00	70	7.8	0.00	70	15.40	2.24	29	4.9
Circles3D36	15.77	0.44	70	7.3	12.04	70	18.50	15.72	34	10.8
Proc8	68.01	-829.0	34	4.6	67.12	2	1.0	68.01	0	1.7
Proc10	-73.51	-1,108.88	197	21.7	-78.81	4	1.0	-73.56	2	1.9
Proc12	-69.51	-1,108.88	234	27.7	-74.81	8	1.0	-69.51	2	2.9
Flay02	37.95	28.28	6	1.0	28.28	6	1.7	37.95	3	1.0
Flay03	48.99	30.98	104	10.7	30.98	108	12.1	41.94	30	9.0
Flay04	54.40	30.98	2,415	234.0	30.98	2,887	288.0	41.69	52	48.0
Clay0203	41,573.30									
Clay0303	26,670.00									
Clay0204	6,545.00									

Improved lower bounds 100%probs

Proposed vs BM: faster 10 out of 12

Proposed vs HR: faster 8 out of 12

Disjunctive Model using EMP-LOGMIP

```
LOGIC EQUATION IMP8; IMP8..  Y('6') -> Y('4')                      ;
LOGIC EQUATION IMP9; IMP9..  Y('7') -> Y('4')                      ;
```

LOGIC PROPOSITIONS

```
* Initialization
 Y.L('1') = 1;
 Y.L('2') = 0;
 Y.L('3') = 1;
 Y.L('4') = 0;
 Y.L('5') = 0;
 Y.L('6') = 0;
 Y.L('7') = 0;
 Y.L('8') = 1;

$ONECHO > '%LM.INFO%'
 DISJUNCTION bigM 50 Y('1') INOUT11 INOUT14 ELSE INOUT12 INOUT13
 DISJUNCTION Y('2') INOUT21 INOUT24 ELSE INOUT22 INOUT23
 DISJUNCTION Y('3') INOUT31 INOUT34 ELSE INOUT32
 DISJUNCTION Y('4') INOUT41 INOUT45 ELSE INOUT42 INOUT43 INOUT44
 DISJUNCTION Y('5') INOUT51 INOUT54 ELSE INOUT52 INOUT53
 DISJUNCTION Y('6') INOUT61 INOUT64 ELSE INOUT62 INOUT63
 DISJUNCTION Y('7') INOUT71 INOUT74 ELSE INOUT72 INOUT73
 DISJUNCTION Y('8') INOUT81 INOUT86 ELSE INOUT82 INOUT83 INOUT84 INOUT85
* optional, if not set LOGMIP will find the modeltype suitable
 MODELTYPE MINLP
$OFFECHO

 OPTION OPTCR = 0, LIMCOL = 0, LIMROW = 0, EMP = LOGMIP;

 MODEL EXAMPLE3  / ALL / ;

 SOLVE EXAMPLE3 USING EMP MINIMIZING PROF   ;
```

Disjunction reformulated using Big-M formulation

DISJUNCTIONS

(Default: Reformulation Using Hull Relaxation)

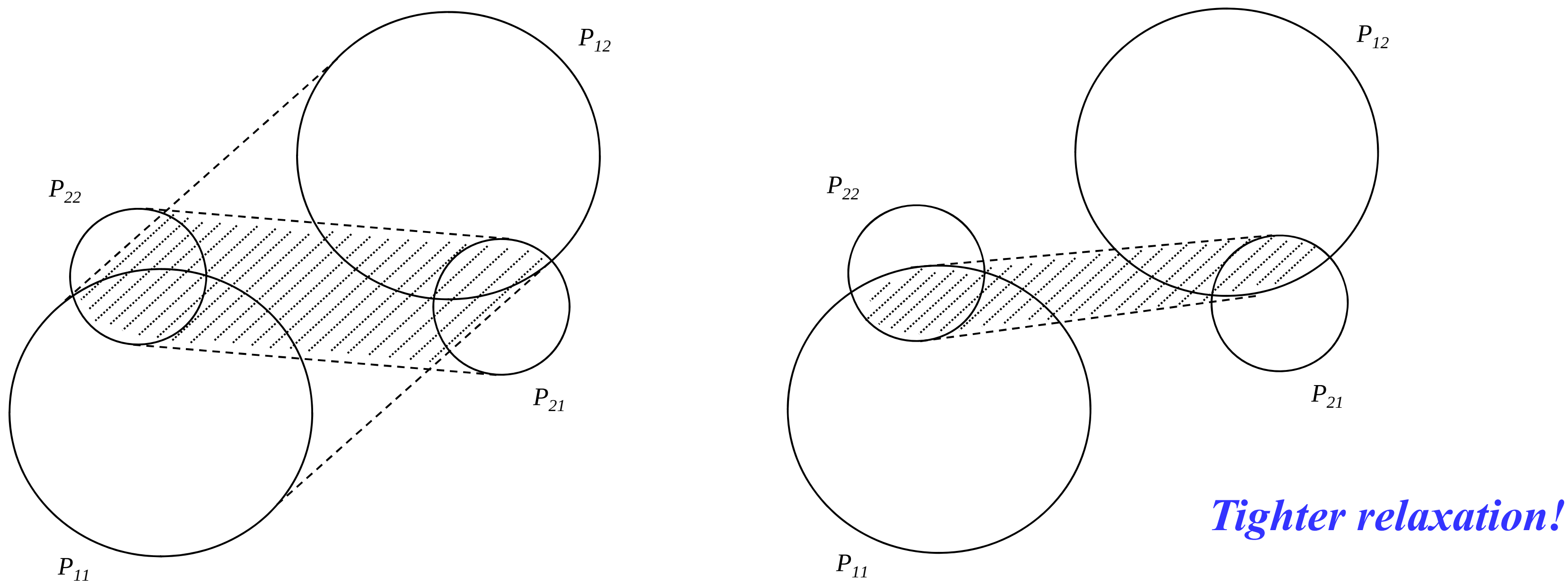
Fragment taken from Logmip 3 (GAMS Library)
EMP= Extended Mathematical Programming

Hierarchy of Relaxations for Convex Disjunctive Programs

Theorem 2.4. *For $i = 1, 2 \ldots k$ let $F_i = \bigcap_{k \in K} S_k$ be a sequence of regular forms of a disjunctive set such that F_i is obtained from F_{i-1} by the application of a basic step, then:*

$$h\text{-}rel(F_i) \subseteq h\text{-}rel(F_{i-1})$$

Illustration: $F_0 = (P_{11} \cup P_{12}) \cap (P_{21} \cup P_{22})$ $\quad F_1 = (P_{11} \cap P_{21}) \cup (P_{11} \cap P_{22}) \cup (P_{12} \cap P_{21}) \cup (P_{21} \cap P_{22})$



No Basic Step Applied => HR

Basic Step Applied => CH

Can we obtain stronger relaxations for MINLP/GDP?

Assume *convexity* and relate *GDP to Disjunctive Programming (DP)* ***Sawaya (2007), Ruiz (2011)***

GDP

$$
\begin{aligned}
\min \quad & Z = f(x) + \textstyle\sum_{k \in K} c_k \\
s.t. \quad & r(x) \le 0 \\
& \bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ g_{ik}(x) \le 0 \\ c_k = \gamma_{ik} \end{bmatrix} \qquad k \in K \\
& \Omega(Y) = True \\
& x^{lo} \le x \le x^{up} \\
& x \in R^n,\ c_k \in R^1,\ Y_{ik} \in \{True, False\}
\end{aligned}
$$

Can we obtain stronger relaxations for MINLP/GDP?

Assume *convexity* and relate *GDP to Disjunctive Programming (DP)* ***Sawaya (2007), Ruiz (2011)***

GDP

$$\min \quad Z = f(x) + \sum_{k \in K} c_k$$

$$s.t. \quad r(x) \leq 0$$

$$\bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ g_{ik}(x) \leq 0 \\ c_k = \gamma_{ik} \end{bmatrix} \quad k \in K$$

$$\Omega(Y) = True$$

$$x^{lo} \leq x \leq x^{up}$$

$$x \in R^n, \; c_k \in R^1, \; Y_{ik} \in \{True, False\}$$

DP

$$\min \quad Z = f(x) + \sum_{k \in K} c_k$$

$$s.t. \quad r(x) \leq 0$$

$$\bigvee_{i \in D_k} \begin{bmatrix} \lambda_{ik} = 1 \\ g_{ik}(x) \leq 0 \\ c_k = \gamma_{ik} \end{bmatrix} \quad k \in K$$

$$A\lambda \geq a \qquad \sum_{i \in D} \lambda_i = 1,$$

$$x^{lo} \leq x \leq x^{up}$$

$$x \in R^n, \; c_k \in R^1, \; \lambda_{ik} \geq 0$$

The integrality of λ is guaranteed

Proposition: GDP and DP have equivalent solutions.