Challenges in the Application of Mathematical Programming in the Enterprise-wide Optimization of Process Industries

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January 17, 2014

Motivation for Enterprise-wide Optimization

Process industry:

Trend to global operations
Pressure for reducing costs, inventories and ecological footprint

⇒ **Major goal: Enterprise-wide Optimization**

Recent research area in Process Systems Engineering:
Grossmann (2005); Varma, Reklaitis, Blau, Pekny (2007)

A major challenge: optimization models and solution methods

Enterprise-wide Optimization (EWO)

EWO involves optimizing the operations of R&D, material supply, manufacturing, distribution of a company to reduce costs, inventories, ecological footprint and to maximize profits, responsiveness .

Key element: Supply Chain

Example: petroleum industry

Wellhead

Trading

Transfer of Crude

Refinery Processing

Schedule Products

Transfer of Products

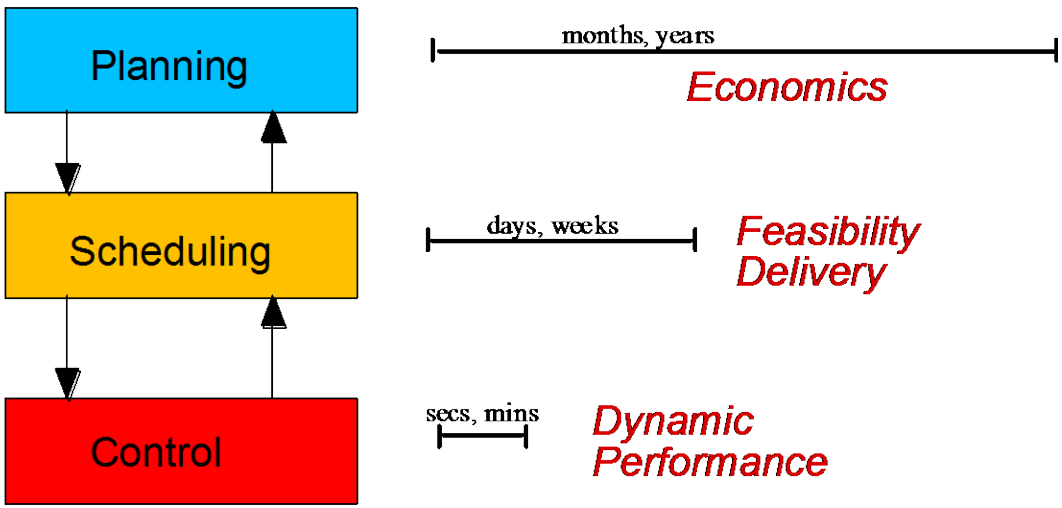
Terminal Loading

Pump

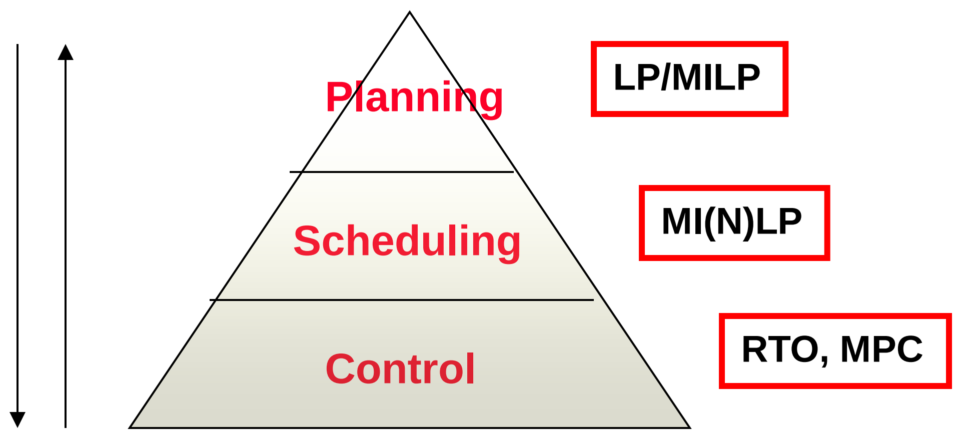
Key issues:

I. Integration of <u>planning, scheduling and control</u>

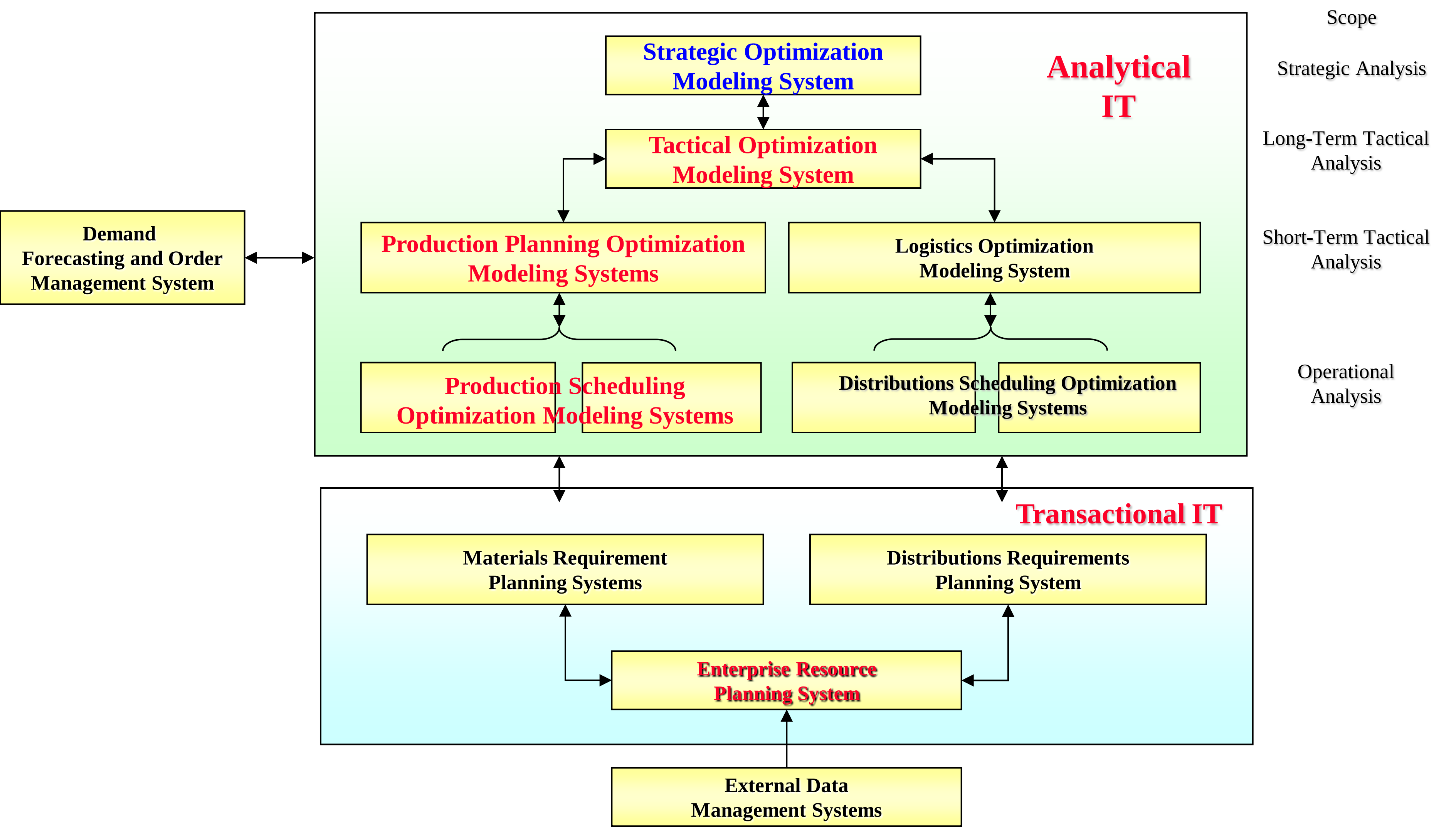
<u>Multiple time scales</u>



<u>Multiple models</u>



II. Integration of information and models/solution methods



Source: Tayur, et al. [1999]

Optimization Modeling Framework: Mathematical Programming

$$\min Z = f(x, y) \quad \text{Objective function}$$

$$s.t. \quad h(x, y) = 0$$

$$g(x, y) \leq 0 \quad \text{Constraints}$$

$$x \in R^n, \quad y \in \{0,1\}^m$$

MINLP: Mixed-integer Nonlinear Programming Problem

Linear/Nonlinear Programming (LP/NLP)

$$\min Z = f(x)$$
$$s.t. \quad h(x) = 0$$
$$g(x) \le 0$$
$$x \in R^n$$

LP Codes:
CPLEX, XPRESS, GUROBI, XA

Very large-scale models
Interior-point: solvable polynomial time

NLP Codes:
CONOPT *Drud (1998)*
IPOPT *Waechter & Biegler (2006)*
Knitro *Byrd, Nocedal, Waltz (2006)*
MINOS *Murtagh, Saunders (1995)*
SNOPT *Gill, Murray, Saunders(2006)*
BARON *Sahinidis et al. (1998)*
Couenne *Belotti, Margot (2008)*
} Global Optimization

Large-scale models
RTO: *Marlin, Hrymak (1996)*
Zavala, Biegler (2009)

Issues:
Convergence
Nonconvexities

Mixed-integer Linear/Nonlinear Programming (MILP/MINLP)

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

MILP Codes:
CPLEX, XPRESS, GUROBI, XA

Great Progress over last decade despite NP-hard
Planning/Scheduling: *Lin, Floudas (2004)*
Mendez, Cerdá , Grossmann, Harjunkoski (2006)
Pochet, Wolsey (2006)

MINLP Codes:
DICOPT (GAMS) *Duran and Grossmann (1986)*
a-ECP *Westerlund and Petersson (1996)*
MINOPT *Schweiger and Floudas (1998)*
MINLP-BB (AMPL) *Fletcher and Leyffer (1999)*
SBB (GAMS) *Bussieck (2000)*
Bonmin (COIN-OR) *Bonami et al (2006)*
FilMINT *Linderoth and Leyffer (2006)*
BARON *Sahinidis et al. (1998)*
Couenne *Belotti, Margot (2008)*
GLOMIQO *Floudas, Meisner (2011)*
} Global Optimization

New codes over last decade
Leveraging progress in MILP/NLP

Issues:
Convergence
Nonconvexities
Scalability

Modeling systems

Mathematical Programming

GAMS *(Meeraus et al, 1997)*

AMPL *(Fourer et al., 1995)*

AIMSS *(Bisschop et al. 2000)*

1. Algebraic modeling systems => pure equation models
2. Indexing capability => large-scale problems
3. Automatic differentiation => no derivatives by user
4. Automatic interface with
   LP/MILP/NLP/MINLP solvers

Have greatly facilitated development and implementation of Math Programming models

Generalized Disjunctive Programming (GDP)

Raman, Grossmann (1994)

$$\min Z = \sum_k c_k + f(x)$$

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

$$\bigvee_{j \in J_k} \begin{bmatrix} Y_{jk} \\ g_{jk}(x) \le 0 \\ c_k = \gamma_{jk} \end{bmatrix} \quad k \in K$$

Disjunctions

$$\Omega(Y) = true$$

Logic Propositions

$$x \in R^n, \; c_k \in R^1$$

Continuous Variables

$$Y_{jk} \in \{ true, false \}$$

Boolean Variables

Codes:
LOGMIP **(*GAMS-Vecchietti, Grossmann, 2005*)**
EMP **(*GAMS-Ferris, Meeraus, 2010*)**

Framework for deriving schedling models
Castro, Grossmann (2012)

Optimization Under Uncertainty

Multistage Stochastic Programming

Birge & Louveaux, 1997; Sahinidis, 2004

$$min\ \ z = c^1x^1 + E_{\omega^2}[c^2(\omega)x^2(\omega^2) + \ldots + E_{\omega^N}[c^N(\omega)x^N(\omega^N)]\ldots]$$

s.t.

$$W^1x^1 = h^1$$

$$T^1(\omega)x^1 + W^2x^2(\omega^2) = h^2(\omega)$$

$$\vdots$$

$$T^{N-1}(\omega)x^{N-1}(\omega^{N-1}) + W^Nx^N(\omega^N) = h^N(\omega)$$

$$x^1 \geq 0, x^t(\omega^t) \geq 0, t = 2,\ldots, N-1$$

Exogeneous uncertainties
(e.g. demands)

Special case: two-stage programming (N=2)

x^1 stage 1 ω ***x^2 recourse (stage 2)***

Planning with endogenous uncertainties (e.g. yields, size resevoir, test drug):
Goel, Grossmann (2006), Colvin, Maravelias (2009), Gupta, Grossmann (2011)

Robust Optimization

Major concern: feasibility over uncertainty set

Ben-Tal et al., 2009; Bertsimas and Sim (2003)

LP

$$\min_x \; c^T x \;:\; a_i^T x \le b_i, \;\; i = 1, \ldots, m$$

- Ellipsoidal uncertainty:

$$a_i \in \mathcal{E}_i = \{\hat{a}_i + P_i^{1/2} u \;:\; \|u\|_2 \le 1\}$$

Robust scheduling:
Lin, Janak, Floudas (2004); Li, Ierapetritou (2008)

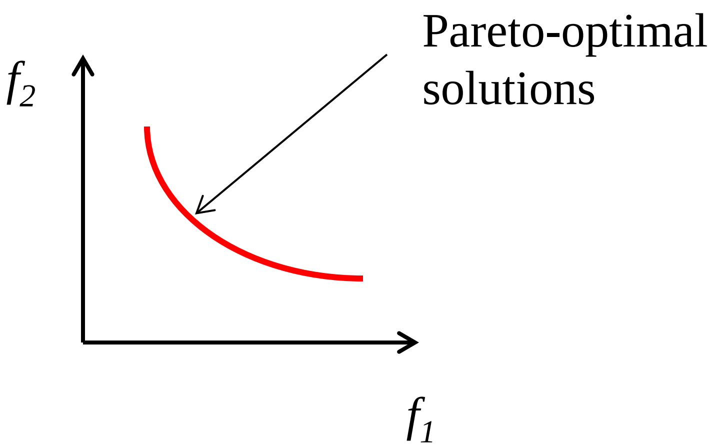
Multiobjective Optimization

$$\min Z = \begin{bmatrix} f_1(x,y) \\ f_2(x,y) \\ \ldots\ldots\ldots \end{bmatrix}$$

$$s.t. \quad h(x,y) = 0$$

$$g(x,y) \le 0$$

$$x \in R^n, \quad y \in \{0,1\}^m$$



ε-constraint method: Ehrgott (2000)

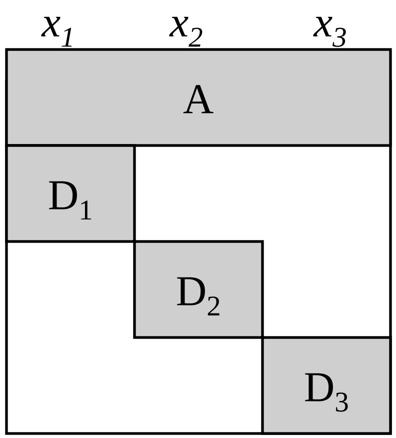
Parametric programming: Pistikopoulos, Georgiadis and Dua (2007)

Decomposition Techniques

Lagrangean decomposition

Geoffrion (1972) Guinard (2003)

Complicating Constraints



complicating constraints

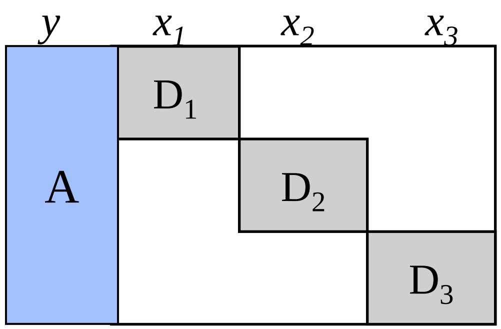
$$\max \; c^T x$$
$$st \;\; Ax = b$$
$$D_i x_i = d_i \;\; i = 1,..n$$
$$x \in X = \{x \mid x_i, i = 1,..n, \mid x_i \geq 0\}$$

Widely used in EWO

Benders decomposition

Benders (1962), Magnanti, Wing (1984)

Complicating Variables



complicating variables

$$\max \; a^T y + \sum_{i=1,..n} c_i^T x_i$$
$$st \;\; Ay + D_i x_i = d_i \;\; i = 1,..n$$
$$y \geq 0, \; x_i \geq 0, \, i = 1,..n$$

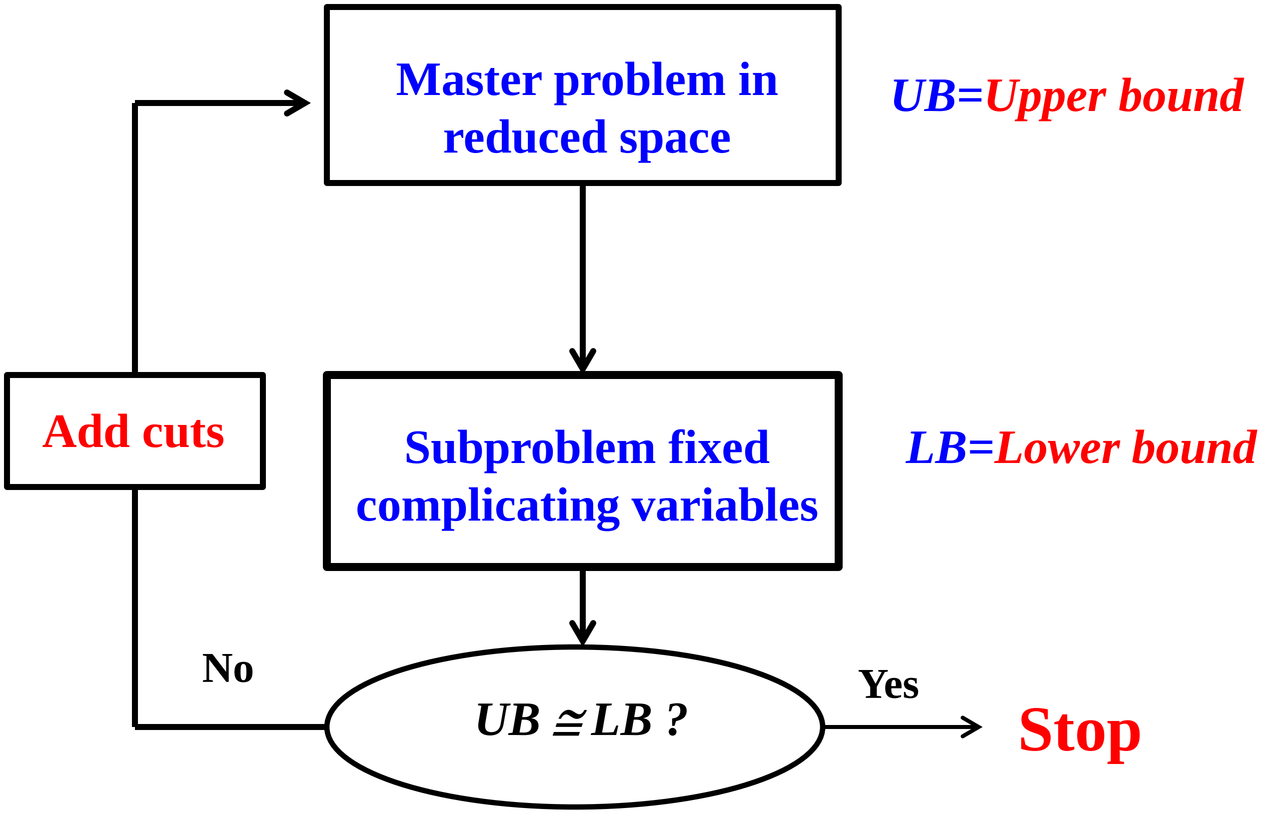
Applied in 2-stage Stochastic Programming

Decomposition Techniques *(cont.)*

Bi-level decomposition

Tailor-made Benders

Iyer, Grossmann (1998)



Institute for Complex Engineered Systems

PITA Project

Special industrial interest group in CAPD:
"Enterprise-wide Optimization for Process Industries"

http://egon.cheme.cmu.edu/ewocp/

Multidisciplinary team:
Chemical engineers, Operations Research, Industrial Engineering

Researchers:

Carnegie Mellon:	**Ignacio Grossmann (ChE)**
	Larry Biegler (ChE)
	Nicola Secomandi (OR)
	John Hooker (OR)
Lehigh University:	**Katya Scheinberg (Ind. Eng)**
	Larry Snyder (Ind. Eng.)
	Jeff Linderoth (Ind. Eng.)

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Projects and case studies with partner companies: "Enterprise-wide Optimization for Process Industries"

ABB: *Optimal Design of Supply Chain for Electric Motors*
Contact: Iiro Harjunkoski — *Ignacio Grossmann, Analia Rodriguez, Yonheng Jiang*

Air Liquide: *Optimal Coordination of Production and Distribution of Industrial Gases*
Contact: Jean Andre, Jeffrey Arbogast — *Ignacio Grossmann, Pablo Marchetti*

Braskem: *Optimal production and scheduling of polymer production*
Contact: Rita Majewski, Wiley Bucey — *Ignacio Grossmann, Pablo Marchetti*

Dow: *Optimal Design of Supply Chains under Disruptions*
Contact: John Wassick — *Ignacio Grossmann, Pablo Garcia-Guerrero*

Dow: *Optimal Operation of Reliable Integrated Sites*
Contact: John Wassick, Anshul Agrawal — *Ignacio Grossmann, Bruno Calfa*

Dow: *Financial Risk with Discrete Event Simulation*
Contact: Bikram Shards, Scott Bury — *Nikolaos Sahinidis, Sayit Amaran*

Dow: *Batch Scheduling and Dynamic Optimization*
Contact: Carlos Villa — *Larry Biegler, Yisu Nie*

Ecopetrol: *Adaptive Process Control*
Contact: Sandra Milena Montagut — *Erik Ydstie, Masoud Golshan*

ExxonMobil: *Global optimization of multiperiod blending networks*
Contact: Myun-Seok Cheon, Kevin Furman, Nick Sawaya — *Ignacio Grossmann, Scott Kolodziej, Francisco Trespalacios*

ExxonMobil: *Design and planning of oil and gasfields with fiscal constraints*
Contact: Bora Tarhan — *Ignacio Grossmann, Vijay Gupta*

Mitsubishi: *Optimization of power flows*
Contact: Arvind Raghunathan — *Larry Biegler, Ajit Gopalakrishnan*

Petrobras: *Nonlinear Integrated Model for Operational Planning of Multi-Site Refineries*
Contact: Lincoln Moro — *Ignacio Grossmann, Breno Menezes*

P&G: *Models for predicting shelf-life of consumer products*
Contact: Ben Weinstein — *Larry Biegler, George Ostace*

Praxair: *Capacity Planning of Power Intensive Networks with Changing Electricity Prices*
Contact: Jose Pinto — *Ignacio Grossmann, Sumit Mitra*

UNILEVER: *Planning and Scheduling of Fast Moving Goods*
Contact: Hans Hogland — *Ignacio Grossmann, Martijn van Elzakker*

Major Issues

-Linear vs Nonlinear models

- The multi-scale optimization challenge

- The uncertainty challenge

- Economics vs performance

- Computational efficiency in large-scale problems

- Commercial vs. Tailored Software

-Linear vs Nonlinear Models

Most EWO problems formulated as MILP

Example: MILP Supply Chain Design Problem
2,001 0-1 vars, 37,312 cont vars, 80,699 constraints

CPLEX 12.2:
MIP Solution: 5,043,251 (160 nodes, 13734 iterations,)

Relative gap: 0.004263 (< 0.5%)

CPU-time: 27 secs!!!

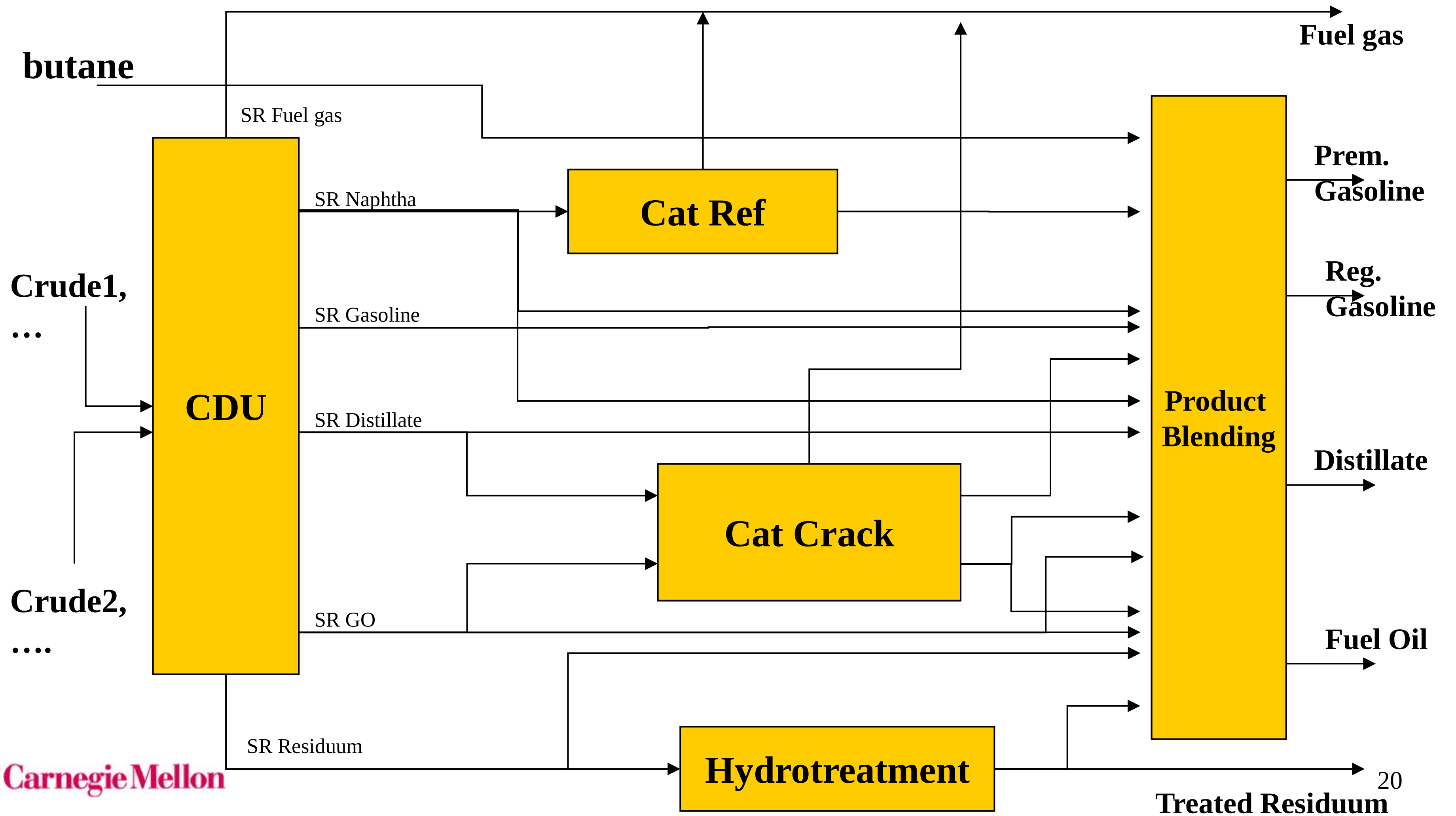
NLP ***required for process models***
MINLP ***required for cyclic scheduling, stochastic inventory, MIDO for integration of control***

Nonlinear CDU Models in Refinery Planning Optimization

Alattas, Palou-Rivera, Grossmann (2010)

Typical Refinery Configuration

(Adapted from Aronofsky, 1978)



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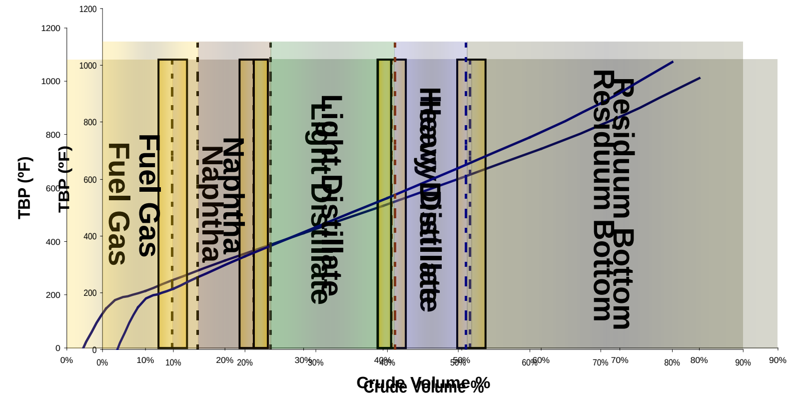
Refinery Planning Models

LP planning models

Fixed yield model
Swing cuts model



Nonlinear FI Model *(Fractionating Index)*

- **FI Model is crude independent**
  - ***FI values are characteristic of the column***
  - ***FI values are readily calculated and updated from refinery data***
- **Avoids more complex, nonlinear modeling equations**
- **Generates cut point temperature settings for the CDU**
- **Adds few additional equations to the planning model**

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 the fixed yield (FY) and swing cut (SC) models
- Economics: maximum profit

FI yields highest profit

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

Model statistics LP vs NLP

- FI model larger number of equations and variables
- Impact on solution time
- ~30% nonlinear variables

	Model	Variables	Equations	Nonlinear Variables	CPU Time	Solver
2 Crude Oil Case	*FY*	128	143		**0.141**	CPLEX
	SC	138	163		**0.188**	
	FI	1202	1225	348	**0.328**	CONOPT

-   Solution large-scale problems:

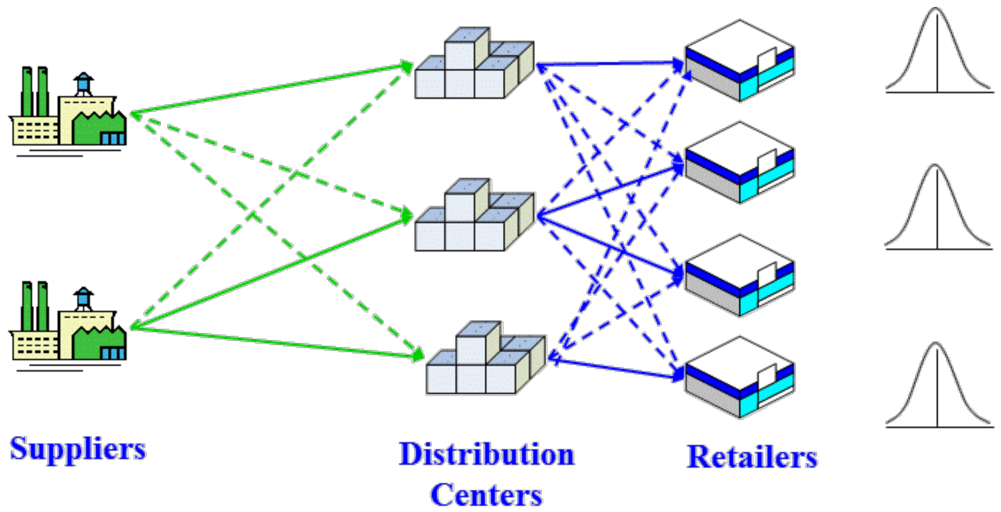
Strategy 1: Exploit problem structure (TSP)

Strategy 2: Decomposition

Strategy 3: Heuristic methods to obtain "good feasible solutions"

Design Supply Chain Stochastic Inventory

You, Grossmann (2008)



- Major Decisions (Network + Inventory)
  - Network: number of DCs and their locations, assignments between retailers and DCs (single sourcing), shipping amounts
  - Inventory: number of replenishment, reorder point, order quantity, safety stock

- Objective: (Minimize Cost)
  - Total cost = DC installation cost + transportation cost + fixed order cost + working inventory cost + safety stock cost

Trade-off: Transportation vs inventory costs

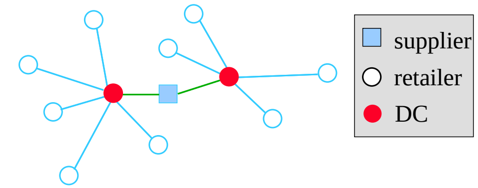
INLP Model Formulation

$$\min \sum_{j \in J} f_j X_j$$ DC installation cost

$$+ \beta \sum_{j \in J} \sum_{i \in I} d_{ij} \chi \mu_i Y_{ij}$$ DC – retailer transportation

$$+ \sum_{j \in J} \sqrt{2\theta h (F_j + \beta g_j) \sum_{i \in I} \chi \mu_i Y_{ij}} + \beta \sum_{i \in I} \sum_{j \in J} (a_j \chi \mu_i Y_{ij})$$ EOQ

$$+ \sum_{j \in J} (\theta h z_\alpha \sqrt{\sum_{i \in I} \sigma_i^2 L_i Y_{ij}})$$ Safety Stock

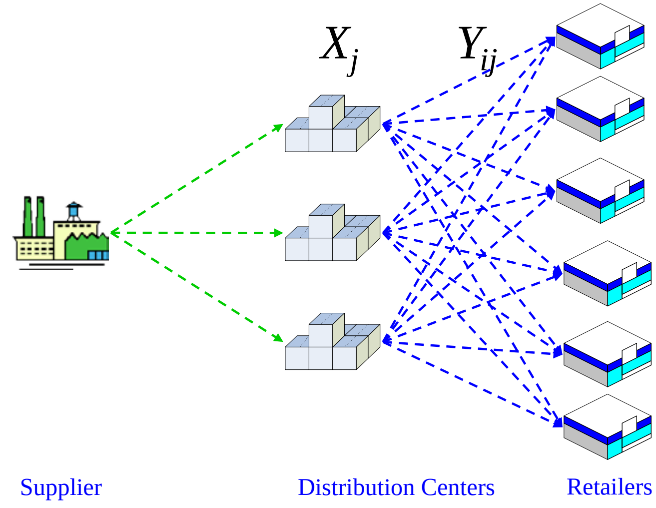


$$\text{s.t.} \quad \sum_{j \in J} Y_{ij} = 1 \quad , \quad \forall i \in I$$

$$Y_{ij} \le X_j \quad , \quad \forall i \in I, j \in J$$

Assignments

$$X_j, Y_{ij} \in \{0, 1\} \quad , \quad \forall i \in I, j \in J$$



Nonconvex INLP:

1. **Variables Y_{ij} can be relaxed as continuous**
2. **Problem reformulated as MINLP**
3. **Solved by Lagrangean Decomposition (by distribution centers)**

Model Properties

- Variables Y_{ij} can be relaxed as continuous variables (MINLP)
  - Local or global optimal solution always have all Y_{ij} at integer
  - If $h=0$, it reduces to an "uncapacitated facility location" problem
  - NLP relaxation is very effective (usually return integer solutions)

$$\min \quad \sum_{j \in J} f_j X_j + \sum_{i \in I} \sum_{j \in J} \hat{d_{ij}} Y_{ij} + \sum_{j \in J} K_j \underbrace{\sqrt{\sum_{i \in I} \mu_i Y_{ij}}}_{Z1_j} + \sum_{j \in J} q \underbrace{\sqrt{\sum_{i \in I} \hat{\sigma_i}^2 Y_{ij}}}_{Z2_j}$$

Avoid unbounded gradient

$$\text{s.t.} \quad \sum_{j \in J} Y_{ij} = 1 \quad , \quad \forall i \in I$$

$$Y_{ij} \le X_j \quad , \quad \forall i \in I, j \in J$$

$$Y_{ij} \ge 0 \quad , \quad \forall i \in I, j \in J$$

$$X_j, \in \{0, 1\} \quad , \quad \forall j \in J$$

Non-convex MINLP

$$\text{where } \hat{d_{ij}} = \beta \mu_i (d_{ij} + a_j), \ \hat{\sigma_i}^2 = L\sigma_i^2 \ K_j = \sqrt{2\theta h (F_j + \beta g_j)}, \ q = \theta h z_\alpha$$

Algorithm 1 – MINLP Heuristic

- MINLP Heuristic Method
  - Solve the convex relaxation (MILP), using secant for convex envelope
  - Use optimal value of X and Y variables as initial point, solve the reformulated problem with an MINLP solver (BARON, Dicopt, etc.)

$$\min \quad \sum_{j\in j} \left\{ f_j X_j + \left(\sum_{i\in I} \hat{d_{ij}} Y_{ij}\right) + K_j Z1_j + q \ Z2_j \right\}$$

$$\text{s.t.} \quad \sum_{j\in J} Y_{ij} = 1 \quad , \quad \forall i \in I$$

$$Y_{ij} \le X_j \quad , \quad \forall i \in I, j \in J$$

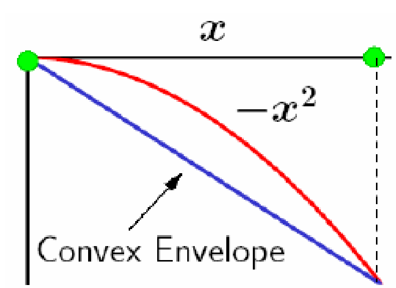
$$Y_{ij} \ge 0 \quad , \quad \forall i \in I, j \in J$$

$$X_j, \in \{0,1\} \quad , \quad \forall j \in J$$

$$-Z1_j^2 + \sum_{i\in I} \mu_i Y_{ij} \le 0 \quad , \quad \forall j \in J$$

$$-Z2_j^2 + \sum_{i\in I} \hat{\sigma}_i{}^2 Y_{ij} \le 0 \quad , \quad \forall j \in J$$

$$Z1_j \ge 0, \ Z2_j \ge 0 \quad , \quad \forall j \in J$$



Convex Relaxation ⟹

$$-\sqrt{\sum_{i\in I} \mu_i} \cdot Z1_j + \sum_{i\in I} \mu_i Y_{ij} \le 0 \quad , \quad \forall j \in J$$

$$-\sqrt{\sum_{i\in I} \hat{\sigma}_i{}^2} \cdot Z2_j + \sum_{i\in I} \hat{\sigma}_i{}^2 Y_{ij} \le 0 \quad , \quad \forall j \in J$$

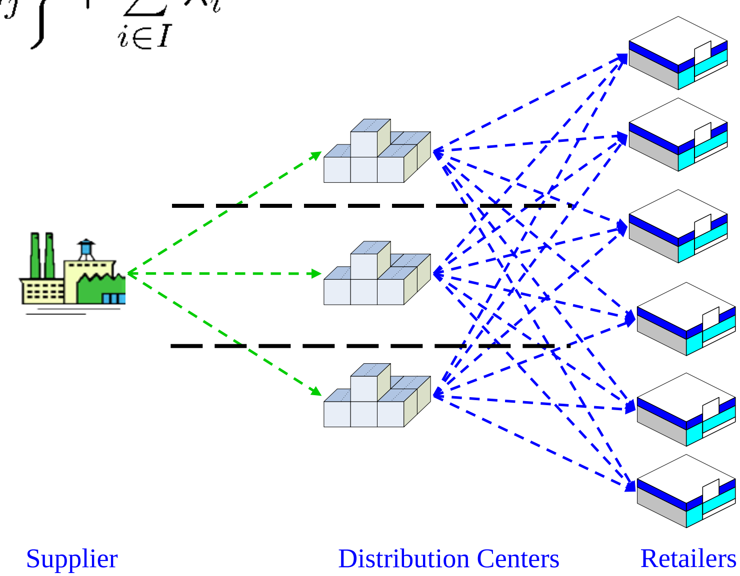
Algorithm 2 - Lagrangean Relaxation

- Lagrangean Relaxation (LR) and Decomposition
  - LR: dualizing the single sourcing constraint: $\sum_{j\in J} Y_{ij} = 1, \forall i \in I$
  - Spatial Decomposition: decompose the problem for each potential DC *j*
  - Implicit constraint: at least one DC should be installed, $\sum_{j\in J} X_j \geq 1$
    - Use a special case of LR subproblem that X_j=1

$$\min \quad \sum_{j\in j} \left\{ f_j X_j + \sum_{i\in I} (\hat{d_{ij}} - \lambda_i) Y_{ij} + K_j Z1_j + q \ Z2_j \right\} + \sum_{i\in I} \lambda_i$$

$$\begin{aligned}
\text{s.t.} \quad & Y_{ij} \leq X_j \quad , && \forall j \in J, \ i \in I \\
& Y_{ij} \geq 0 \quad , && \forall j \in J, \ i \in I \\
& X_j, \in \{0,1\} \quad , && \forall j \in J \\
& -Z1_j^2 + \sum_{i\in I} \mu_i Y_{ij} \leq 0 \quad , && \forall j \in J \\
& -Z2_j^2 + \sum_{i\in I} \hat{\sigma_i}^2 Y_{ij} \leq 0 \quad , && \forall j \in J \\
& Z1_j \geq 0, \ Z2_j \geq 0 \quad , && \forall j \in J
\end{aligned}$$

decompose by DC *j*



Computational Results

- Each instance has the same number of potential DCs as the retailers

150 retailers: MINLP has 150 bin. var., 22,800 cont. var., 22,800 constraints

No. Retailers	β	θ		Lagrangean Relaxation				
				Upper Bound	Lower Bound	Gap	Iter.	Time (s)
88	0.001	0.1		867.55	867.54	**0.001 %**	21	**356.1**
88	0.001	0.5		1230.99	1223.46	**0.615 %**	24	**322.54**
88	0.005	0.1		2284.06	2280.74	**0.146 %**	55	**840.28**
88	0.005	0.5		2918.3	2903.38	**0.514 %**	51	**934.85**
150	0.001	0.5		1847.93	1847.25	**0.037 %**	13	**659.1**
150	0.005	0.1		3689.71	3648.4	**1.132 %**	53	**3061.2**

- Suboptimal solution in 3 out of 6 cases with BARON for 10 hour limit.
  Large optimality gaps

The multi-scale optimization challenge

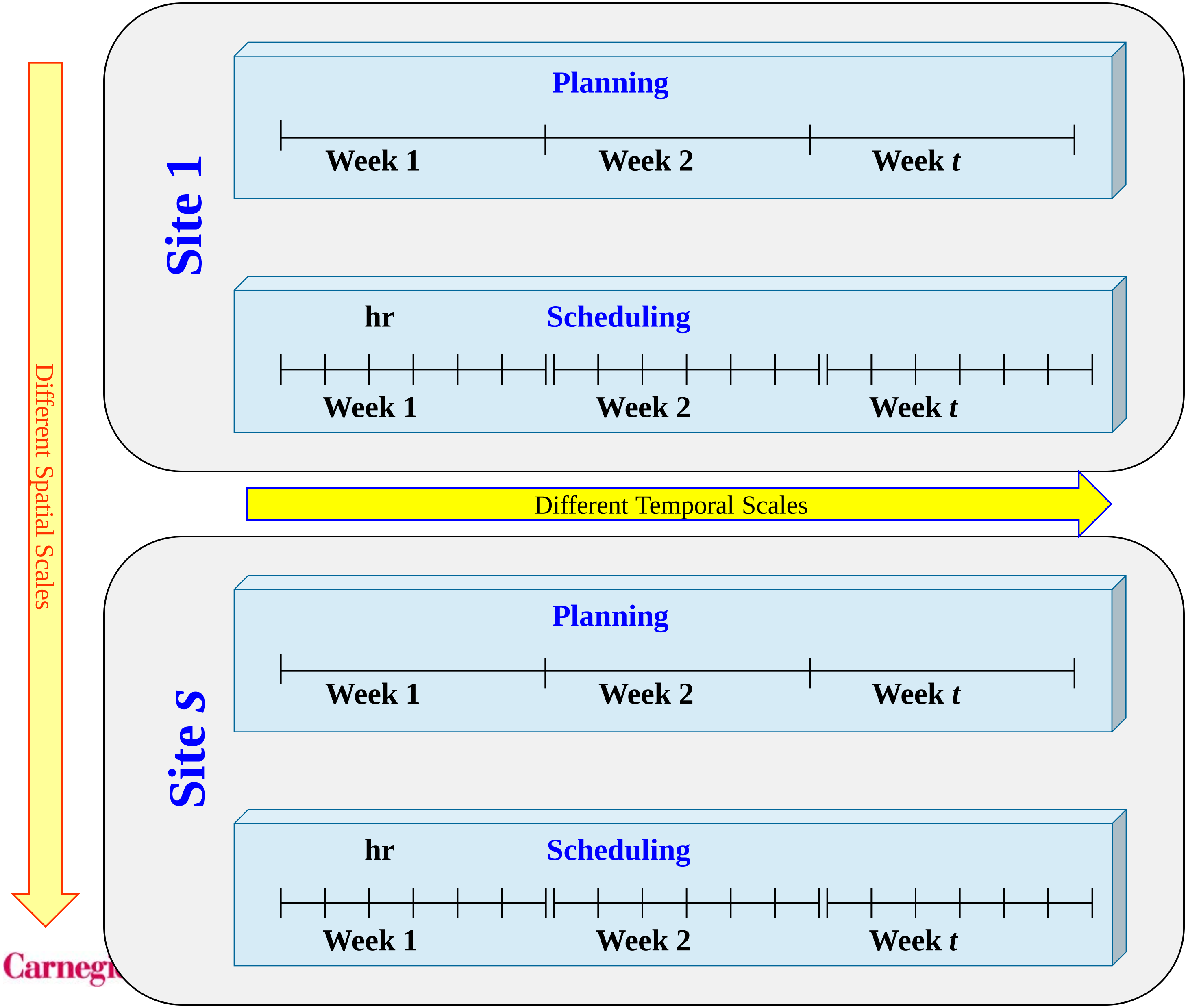
Temporal integration long-term, medium-term and short-term *Bassett, Pekny, Reklaitis (1993), Gupta, Maranas (1999), Jackson, Grossmann (2003), Stefansson, Shah, Jenssen (2006), Erdirik-Dogan, Grossmann (2006), Maravelias, Sung (2009), Li and Ierapetritou (2009), Verderame , Floudas (2010), Salema, Barbosa-Povoa, Novais (2010)*

Spatial integration geographically distributed sites
Gupta, Maranas (2000), Tsiakis, Shah, Pantelides (2001),
Jackson, Grossmann (2003), Terrazas, Trotter, Grossmann (2011)

Decomposition is key: Benders, Lagrangean, bilevel

Multi-site planning and scheduling involves different temporal and spatial scales

Terrazas, Grossmann (2011)



Weekly aggregate production:
- Amounts
- Aggregate sequencing model (TSP constraints)

Detailed operation
- Start and end times
- Allocation to parallel lines

Weekly aggregate production:

Detailed operation

MILP Model

- Objective: Maximize Profit

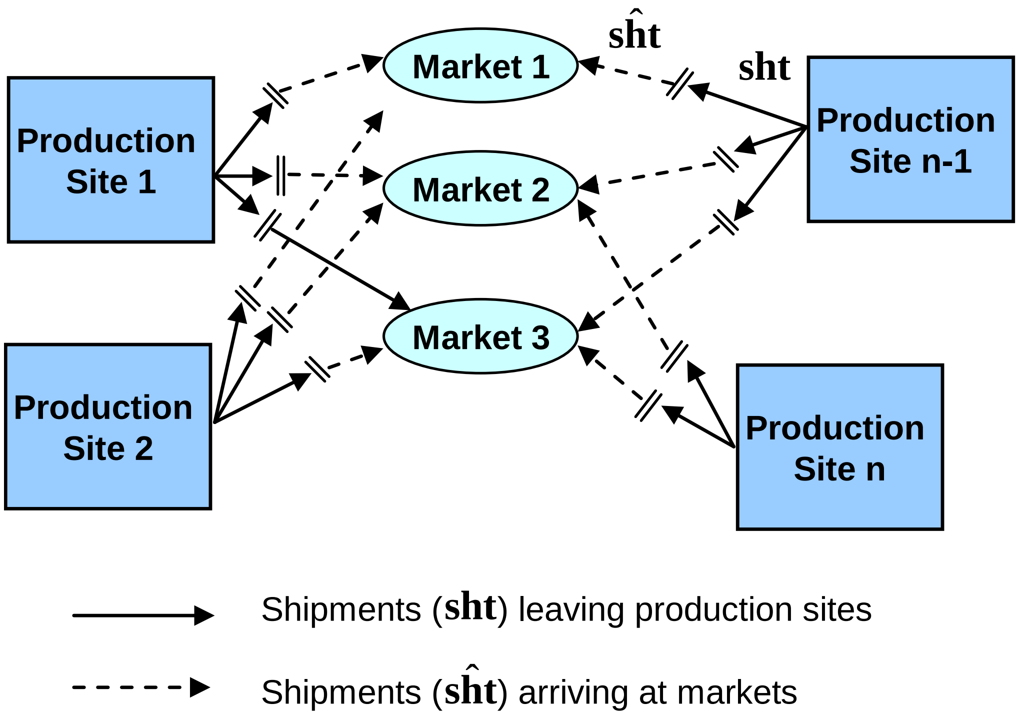
subject to

- Market constraints
  - Balance of sales vs. shipments to markets
- Production constraints
  - Capacity constraints: Limited capacity at each production sites
  - Inventory constraints: Penalties for inventory over or under target
  - Links across periods: a) Carry over inventories from last month
    b) Changeover to first product in next month
  - Time Balances: Task should not take longer than available time
  - Sequencing Constraints: Traveling Salesman Problem Constraints

⇓

Source of complexity of the model: TSP constraints

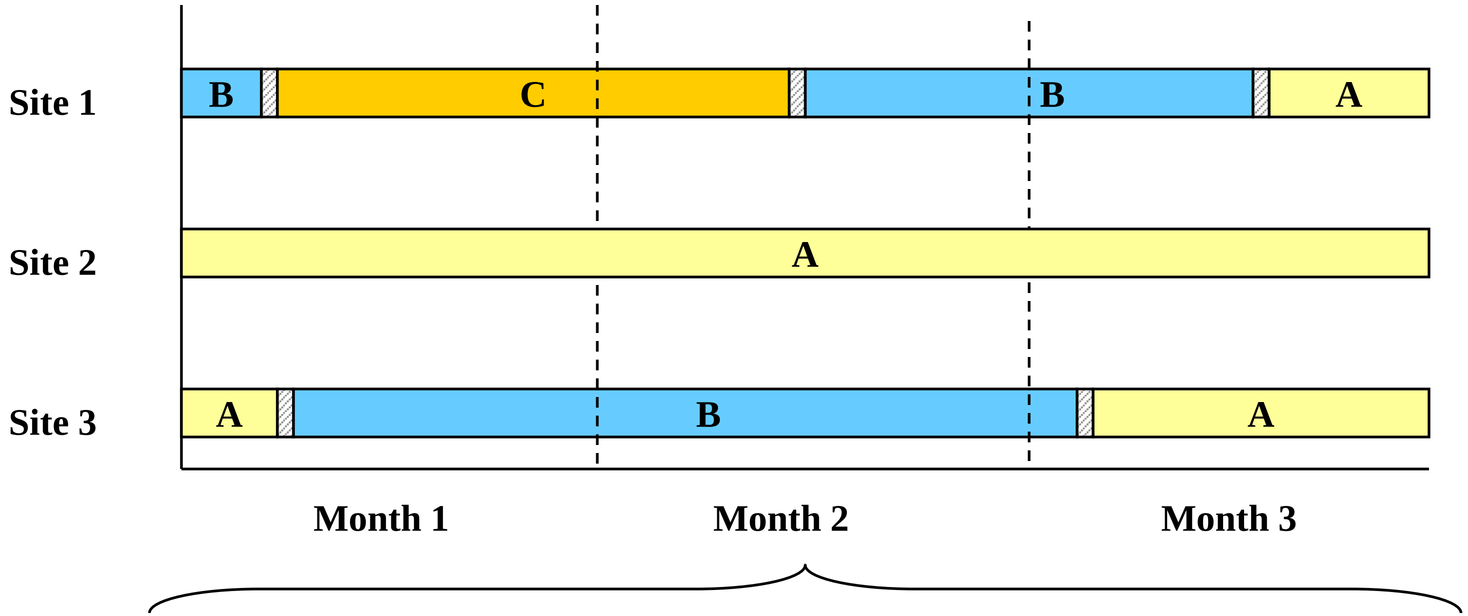
Bilevel decomposition + Lagrangean decomposition

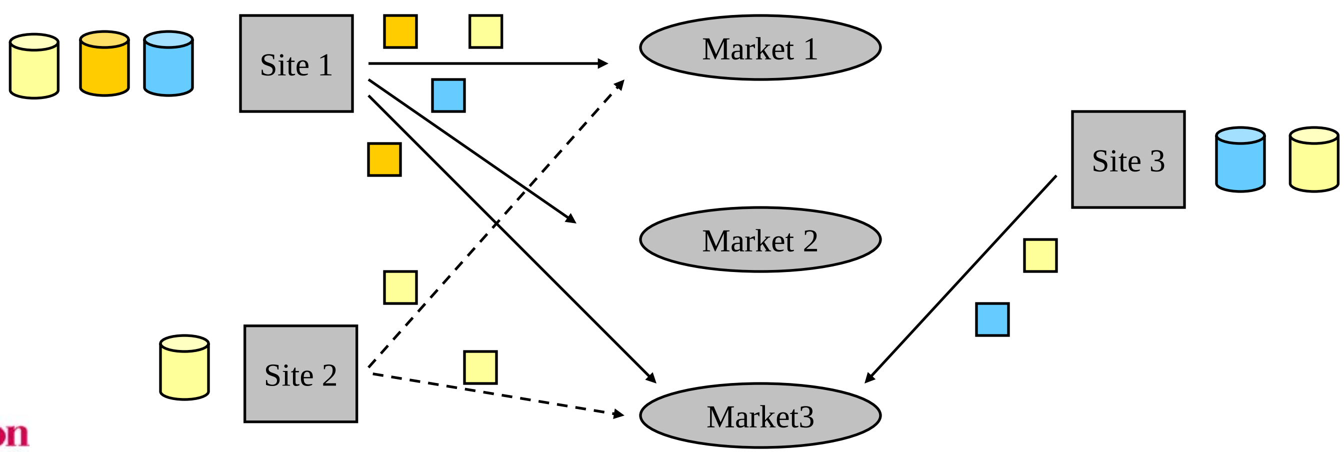


- **Bilevel decomposition**
  - Decouples planning from scheduling
  - Integrates across temporal scale
- **Lagrangean decomposition**
  - Decouples the solution of each production site
  - Integrates across spatial scale

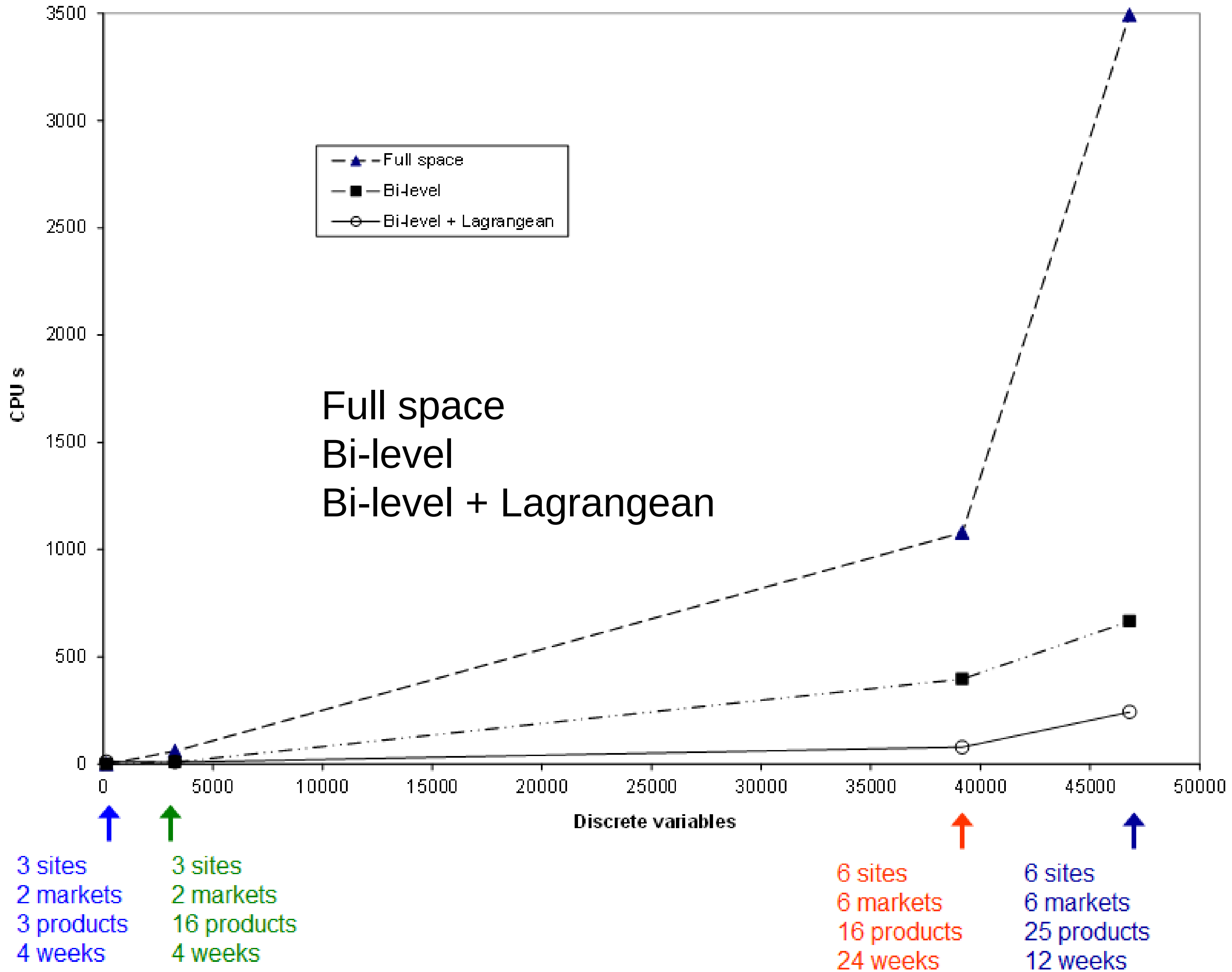
Example: 3 sites, 3 products, 3 months

Profit: $ 2.576 million





Large-scale problems



Carnegie

Integration of operational and strategic decisions for air separation plants

Mitra et al. (2013)

Given:

- Power-intensive plant
- Products $g \in G$ (Storable and Nonstorable)
- Product demands d_g^t for season $t \in T$
- Seasonal electricity prices on an hourly basis $e^{t,h}$, $t \in T$, $h \in H$
- Upgrade options $u \in U$ of existing equipment
- New equipment options $n \in N$
- Additional storage tanks $st \in ST$

Determine:

- Production levels $Pr_g^{t,h}$
- Mode of operation $\tilde{y}_{m,o}^{t,h}$, $y_m^{t,h}$
- Sales $S_g^{t,h}$
- Inventory levels $INV_g^{t,h}$

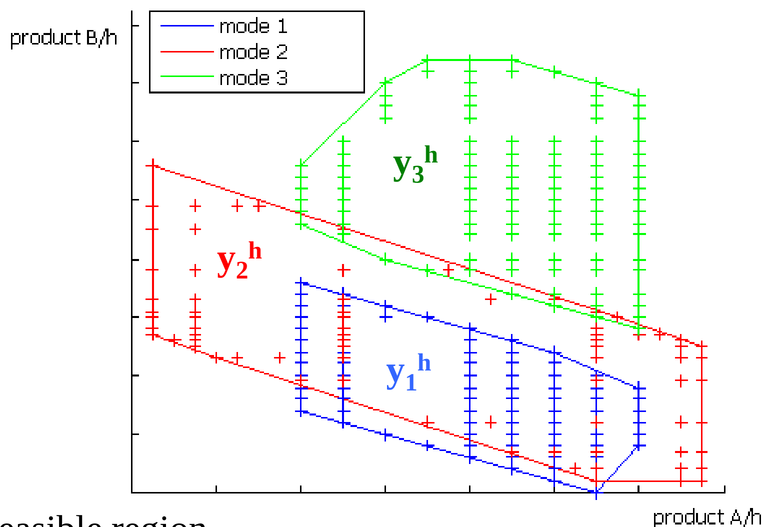
for each season on an hourly basis

- Upgrades for equipment $VU_{m,u}^t$
- Purchase of new equipm. VN_n^t
- Purchase of new tanks $VS_{st,g}^t$

With minimum investment and operating costs

Demand Side Management is part of a complex multi-scale design and operations problem for power-intensive processes.

The operational model is based on a surrogate representation in the product space



Feasible region

Feasible region: projection in product space

Modes: different ways of operating a plant

Mass balances: differences for products with and without inventory

Energy consumption: requires correlation with production levels for each mode

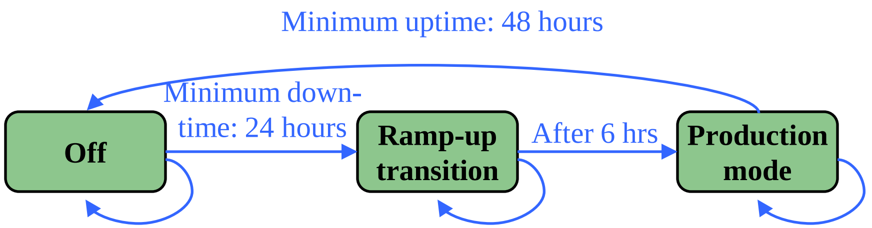
Feasible region

Mass balances

Operational costs

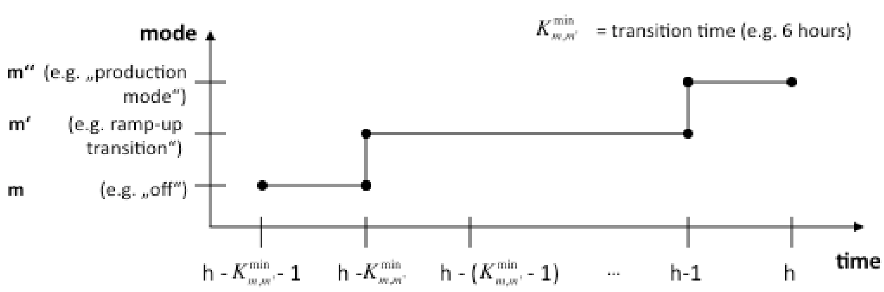
[1] Ierapetritou, M.G.; Wu, D.; Vin, J.; Sweeny P.; Chigirinskiy M. Cost Minimization in an Energy-Intensive Plant Using Mathematical Programming Approaches. Industrial & Engineering Chemistry Research, 41:5262–5277, 2002.
[2] Karwan, K.; Keblis M. Operations planning with real time pricing of a primary input. Computers & Operations Research, 34:848–867, 2007.
[3] Reformulation of disjunction with convex hull according to
Balas, E. Disjunctive Programming and a Hierarchy of Relaxations for Discrete Optimization Problems. SIAM J. Alg. Disc. Meth, 6:466–486, 1985

Transient plant behavior is captured with logic constraints



State diagram for transitions:

- → nodes: states (**modes**) $y^h_{p,m}$
  = different ways of operating a plant
- → arcs = allowed **transitions** $z^h_{p,m,m'}$
  (including constraints, e.g. min. up-/downtime)

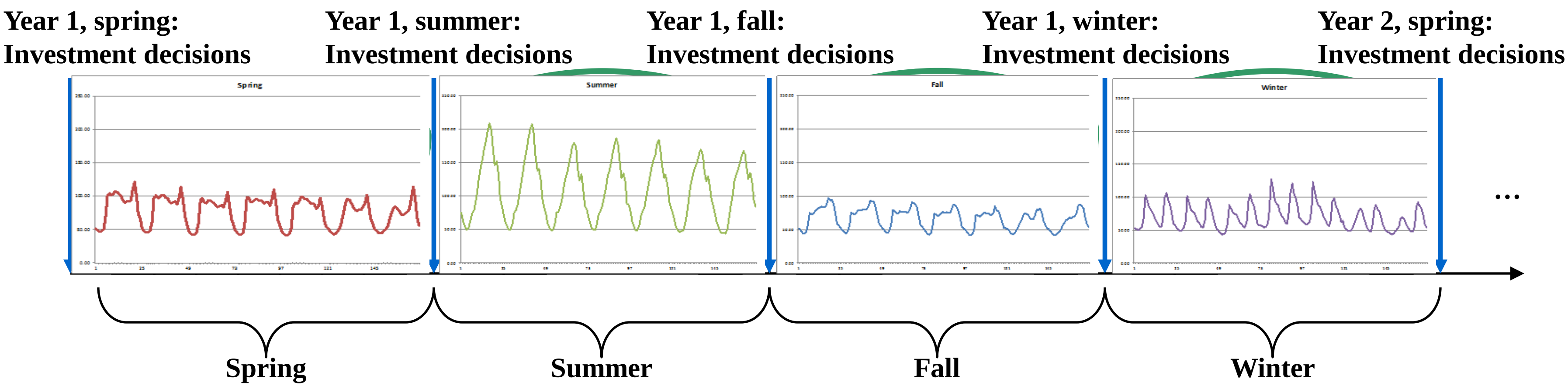


Logic constraints for transitions between different modes

Constraints for transitions within one mode

[*] Derivation of logic constraint using propositional logic according to
Raman, R.; Grossmann, I.E. Modeling and Computational Techniques for Logic Based Integer Programming. Comp. Chem. Eng., 18:563, 1993.

Incorporating design decisions: seasonal variations drive the development of a seasonal model



- Horizon: 5-15 **years**, each year has 4 **periods** (spring, summer, fall, winter)
- Each period is represented by **one week on an hourly basis**
- Varying inputs: **electricity prices, demand data** (here: highly utilized plant)**, configuration slates**
- Each representative week is repeated in a **cyclic** manner (**13** weeks reduced to **1** week)
  (8736 hr vs. 672 hr)
- Connection between periods: Only through investment (design) decisions
- Design decisions are modeled by **discrete equipment sizes**

Multi-scale representation is accomplished by linking operational problem with strategic design decisions

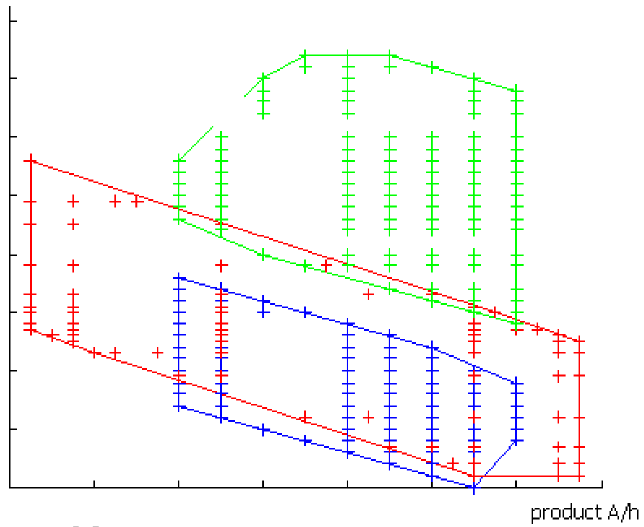


Fig. 1: Feasible region

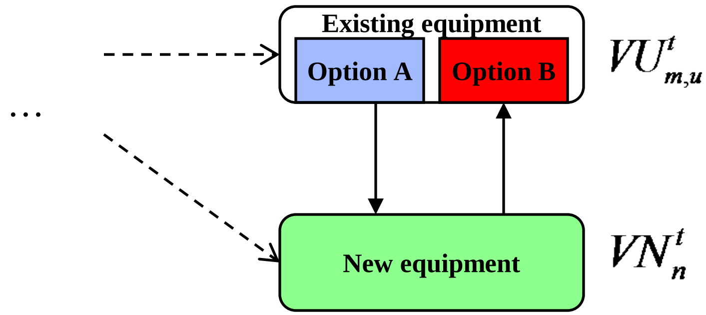


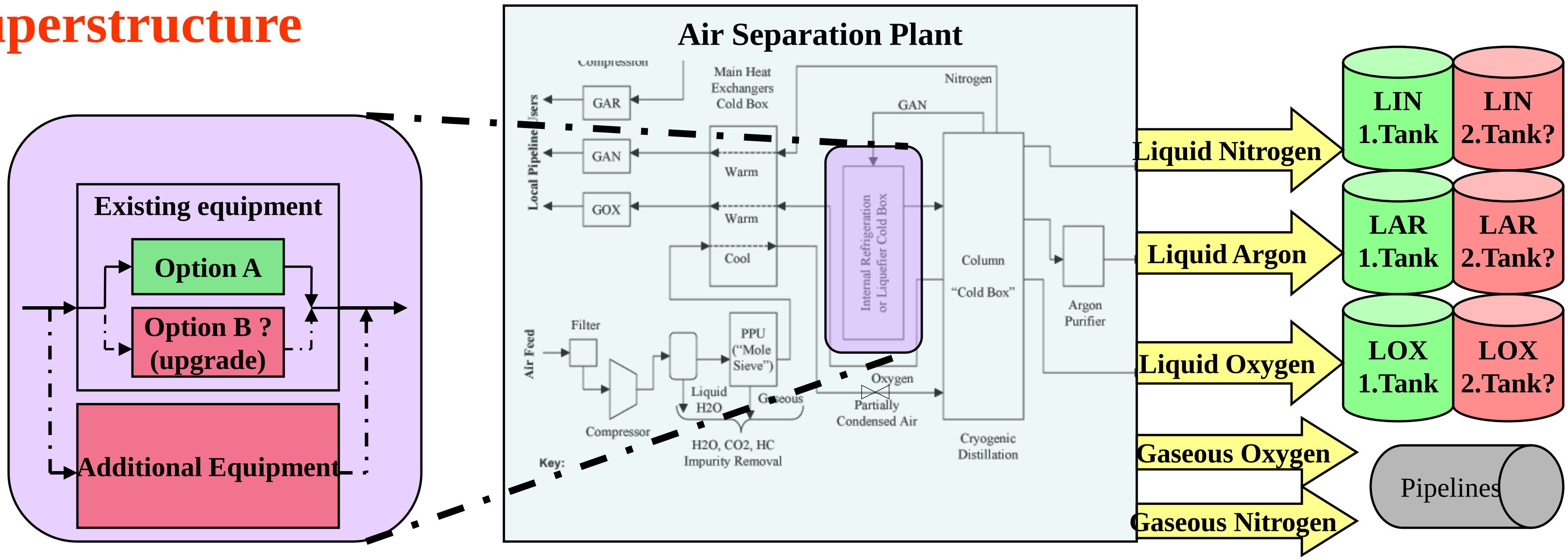
Fig. 2: State graph

Logic constraints for equipment upgrades (polyhedral representation of mode changes)
Logic constraints for additional equipment (additional mode(s) are added to the state graph)
Constraints for additional storage (manipulation of upper bound for inventory)

Objective: minimize investment + operational costs

Retrofitting an air separation plant

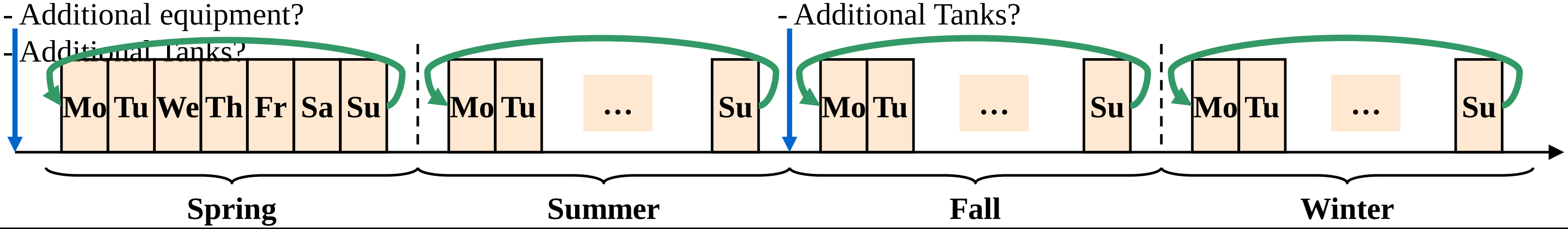
Superstructure



Time

Spring - Investment decisions: (yes/no)
- Option B for existing equipment?
- Additional equipment?
- Additional Tanks?

Fall - Investment decisions: (yes/no)
- Option B for existing equipment?
- Additional equipment?
- Additional Tanks?



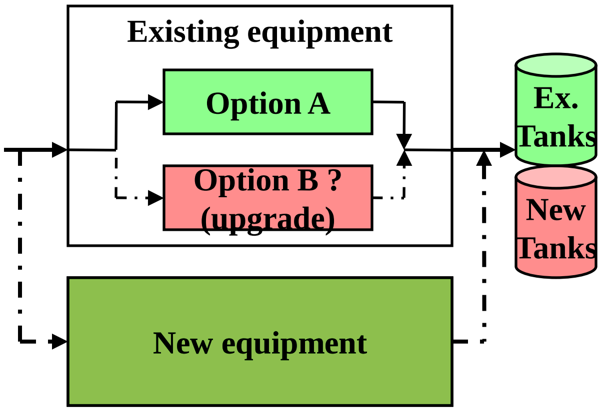


Fig. 1: Flowsheet superstructure

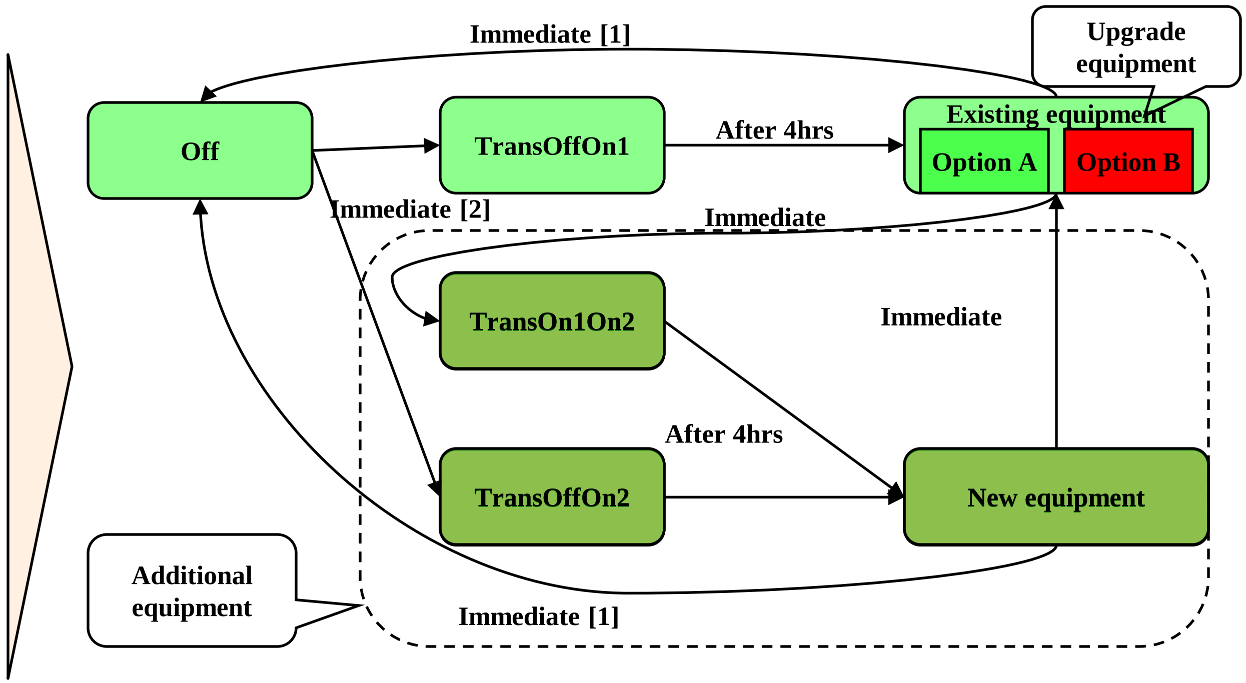
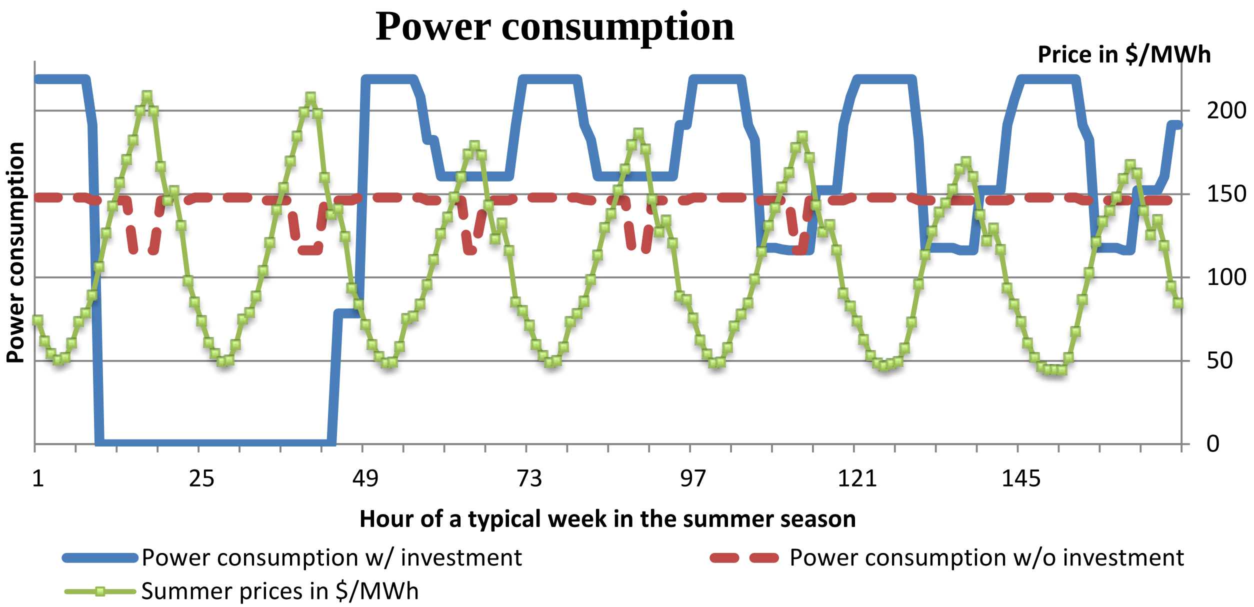
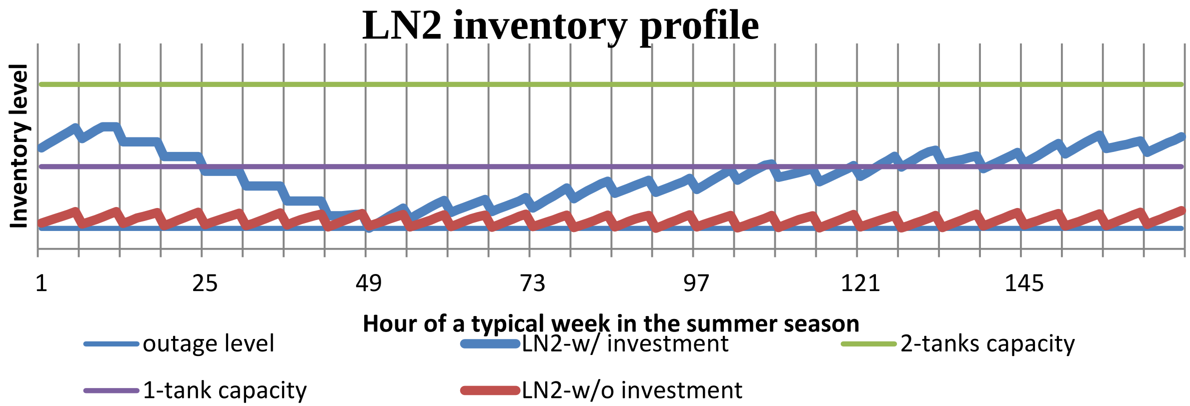


Fig. 2: State graph superstructure

- The resulting MILP has **191,861 constraints** and **161,293 variables (18,826 binary.)**
- Solution time: **38.5 minutes** (GAMS 23.6.2, GUROBI 4.0.0, Intel i7 (2.93GHz) with 4GB RAM

Investments increase flexibility help realizing savings.





Remarks on case study

- **Annualized costs: $5,700k/yr**
- **Annualized savings: $400k/yr**

- Buy new liquefier in the first time period (annualized investment costs: $300k/a)
- Buy additional LN2 storage tank ($25k/a)
- Don't upgrade existing equipment ($200k/a)

- Take-away message on operational level: *Reduce production when prices are high and build up LN2 when prices are low.*
- Utilization of existing equipment: 97%.

Source: CAPD analysis; Mitra, S., I.E. Grossmann, J.M. Pinto and Nikhil Arora, "Integration of strategic and operational decision- making for continuous power-intensive processes", submitted to ESCAPE, London, Juni 2012

- The uncertainty challenge:

Short term uncertainties: **robust optimization**

Computation time comparable to deterministic models

Long term uncertainties: **stochastic programming**

Computation time one to two orders of magnitude larger than deterministic models

Risk Management

Global Sourcing Project with Uncertainties

You, Wassick, Grossmann (2009)

- Given
  - Initial inventory
  - Inventory holding cost and throughput cost
  - Transport times of all the transport links
  - Uncertain production reliability and demands
- Determine
  - Inventory levels, transportation and sale amounts

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

- **Objective: Minimize Cost**

Two-stage stochastic MILP model
1000 scenarios (Monte Carlo sampling)

Chemical ENGINEERING
Carnegie Mellon

MILP Problem Size

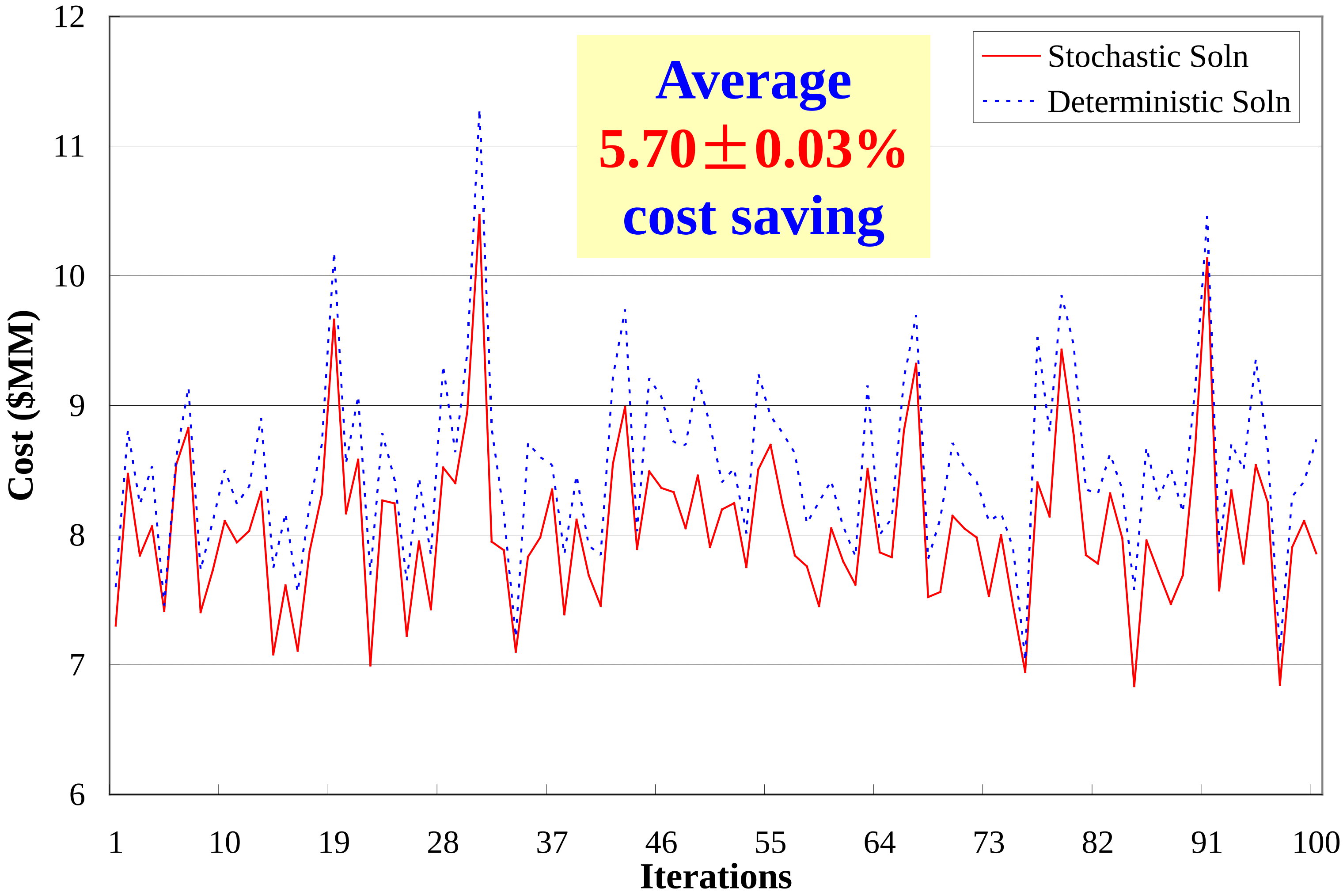
Case Study 1	Deterministic Model
# of Constraints	62,187
# of Cont. Var.	89,014
# of Disc. Var.	7

- Impossible to solve directly
- takes 5 days by using standard L-shaped Benders
- only 20 hours with multi-cut version Benders
- 30 min if using 50 parallel CPUs and multi-cut version

Simulation Results to Assess Benefits Stochastic Model

Risk Management

Stochastic Planner vs Deterministic Planner



Chemical ENGINEERING
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Optimal Development Planning under Uncertainty

ExxonMobil

➢Offshore oilfield having several reservoirs under uncertainty

Tarhan, Grossmann (2010)

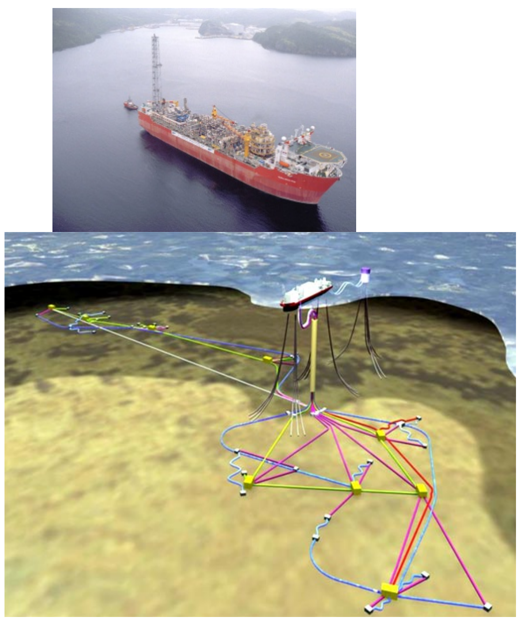
➢Maximize the expected net present value (ENPV) of the project

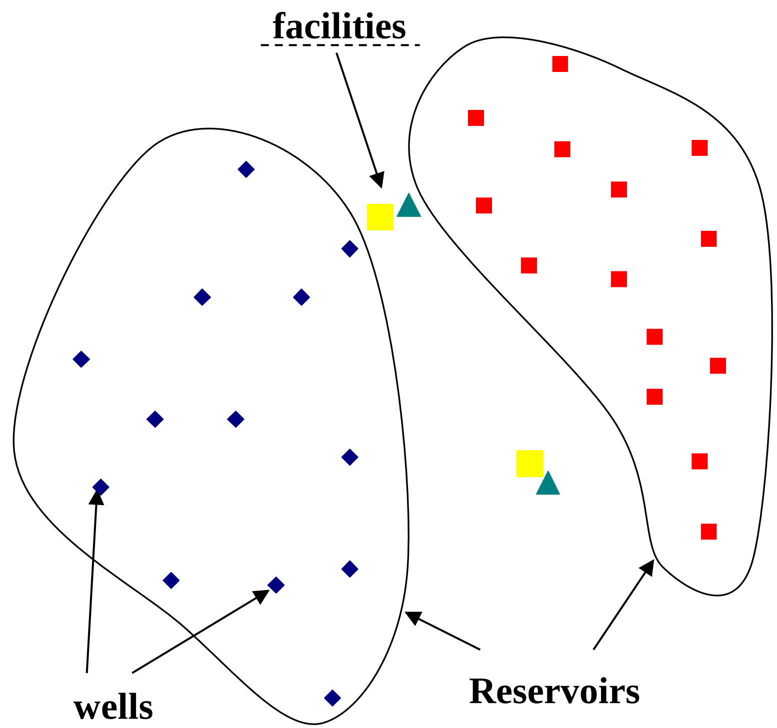
Decisions:

- Number and capacity of TLP/FPSO facilities
- Installation schedule for facilities
- Number of sub-sea/TLP wells to drill
- Oil production profile over time

TLP

FPSO





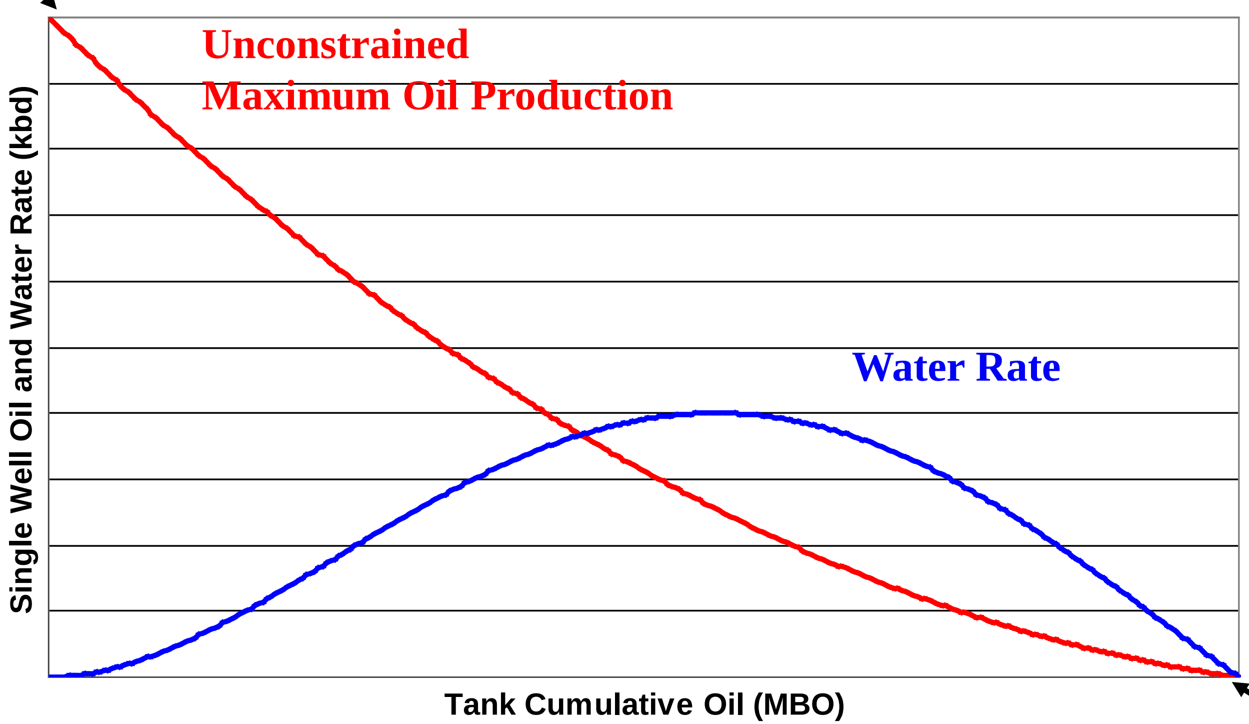
Uncertainty:

- **Initial productivity per well**
- **Size of reservoirs**
- **Water breakthrough time for reservoirs**

Non-linear Reservoir Model

Assumption: **All wells in the same reservoir are identical.**

Initial oil production



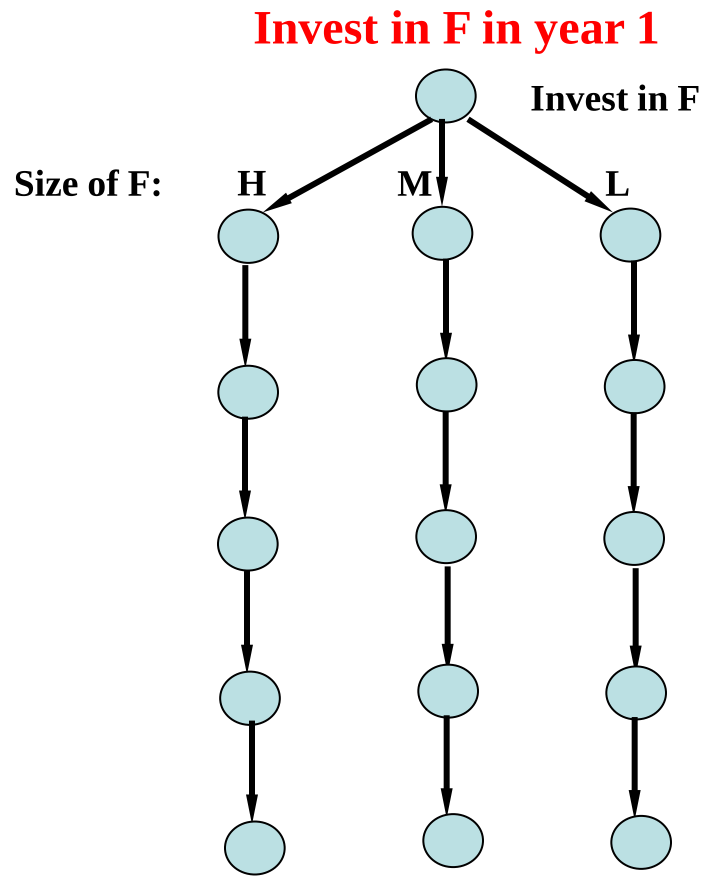
Size of the reservoir

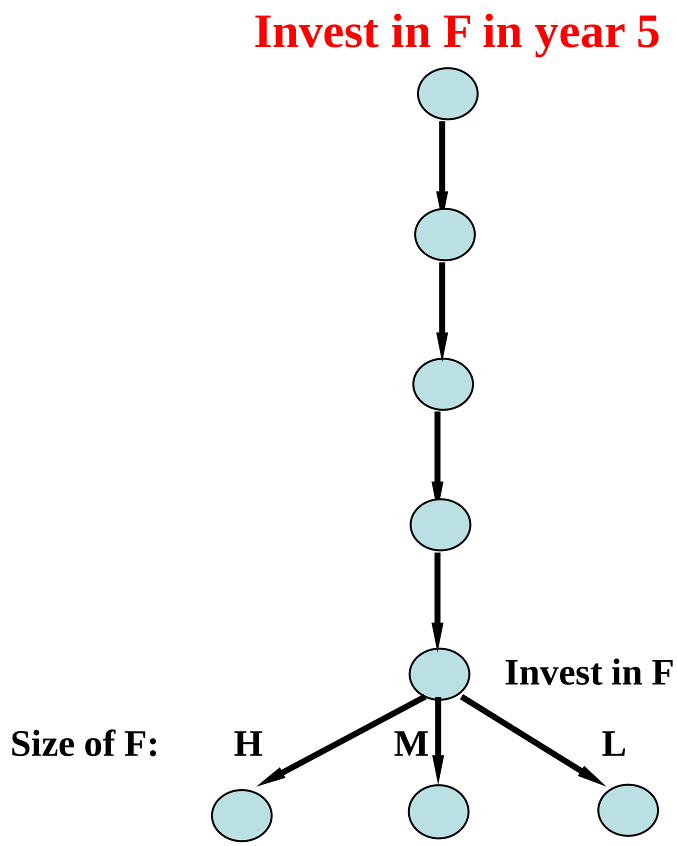
Uncertainty is represented by discrete distributions functions

Decision Dependent Scenario Trees

(Endogeneous uncertainties)

Assumption: Uncertainty in a field resolved as soon as WP installed at field



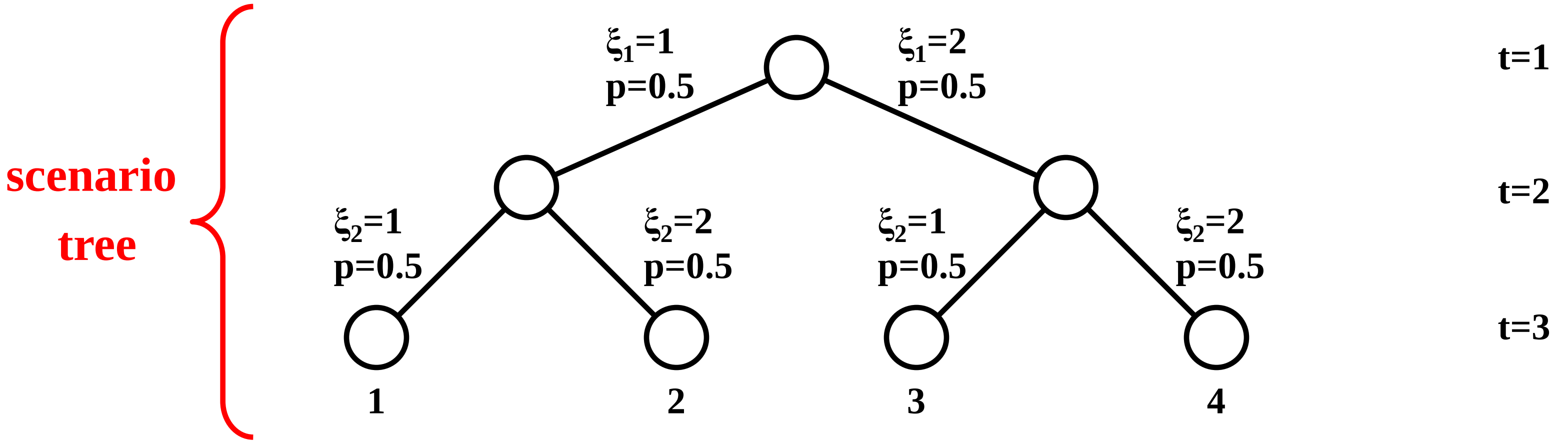


Scenario tree

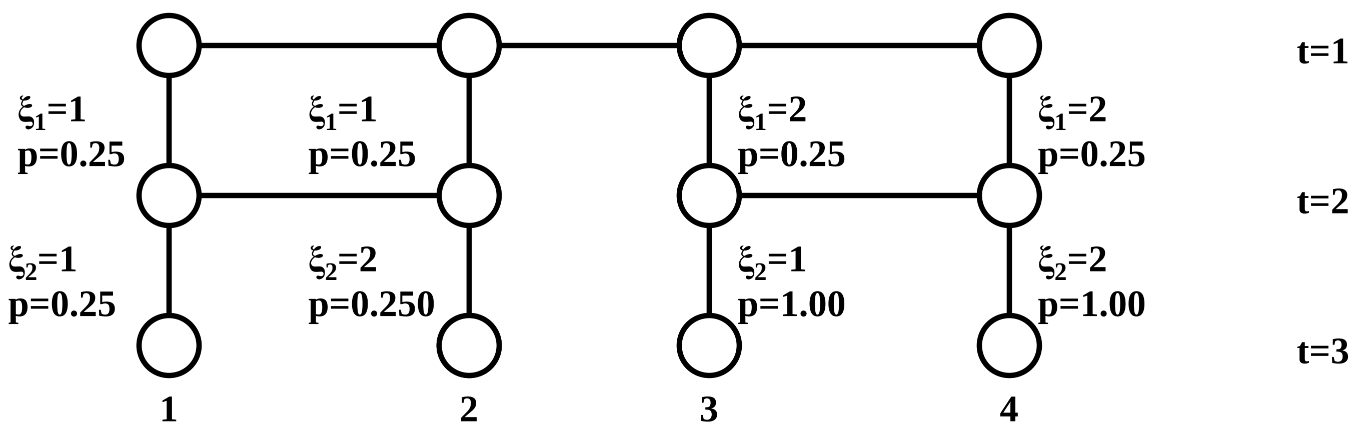
Not unique: Depends on timing of investment at uncertain fields

Central to defining a Stochastic Programming Model

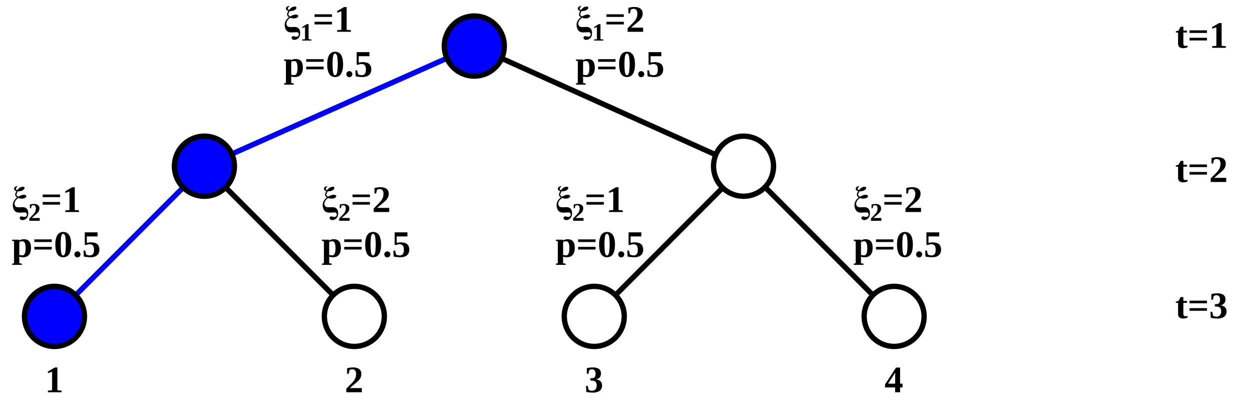
Stochastic Programming



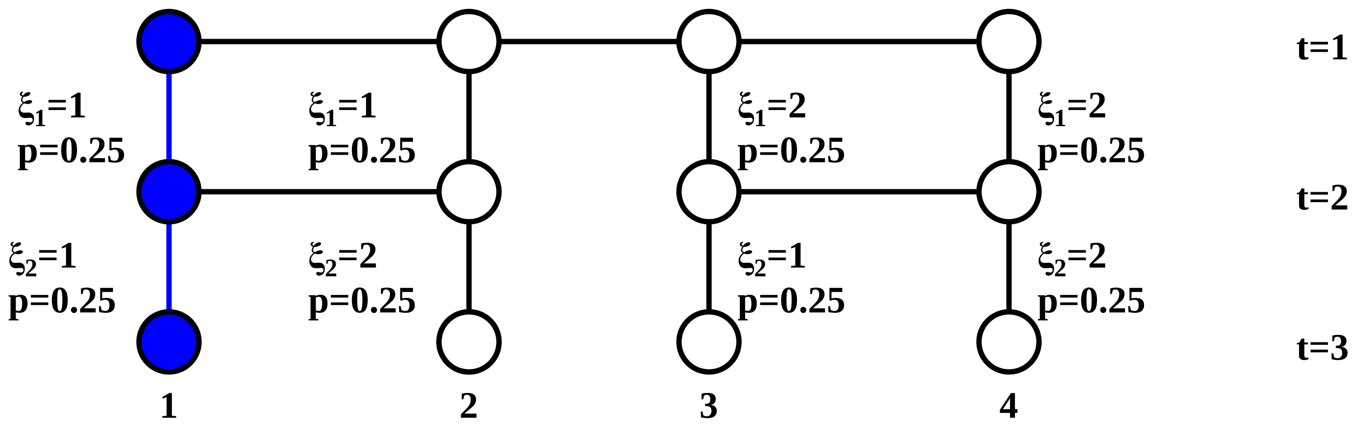
Alternative and equivalent scenario tree structure (Ruszczynski, 1997):



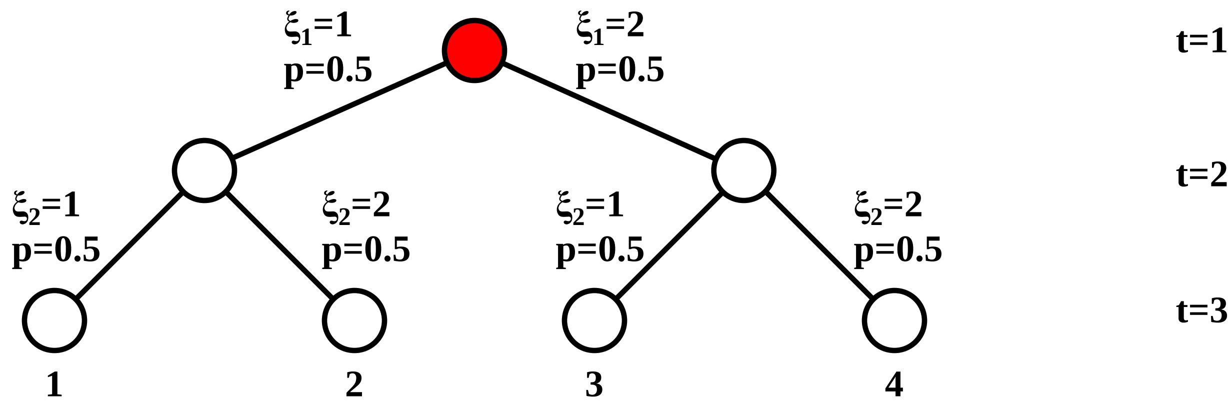
Stochastic Programming



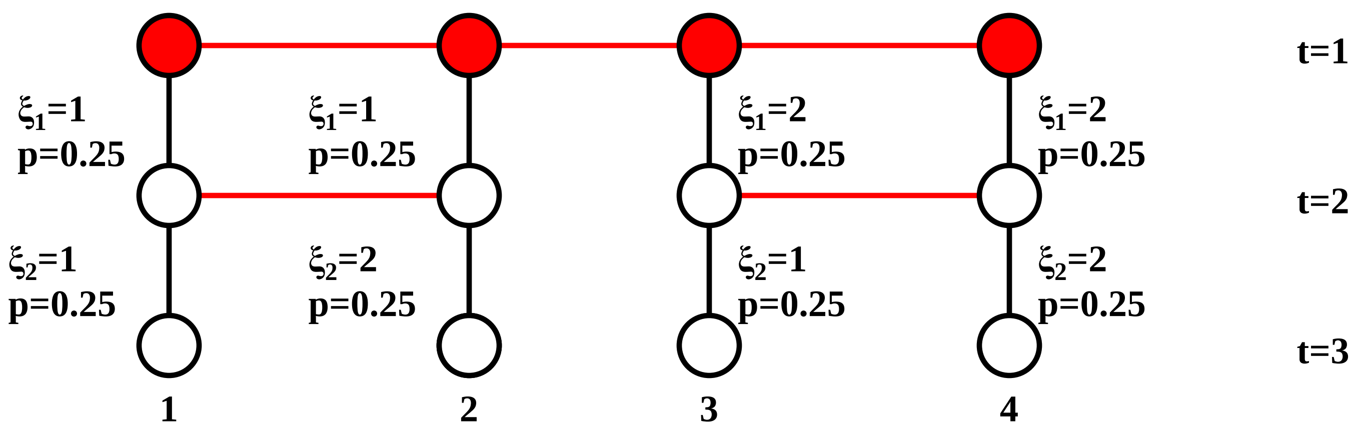
Each scenario is represented by a set of unique nodes



Stochastic Programming

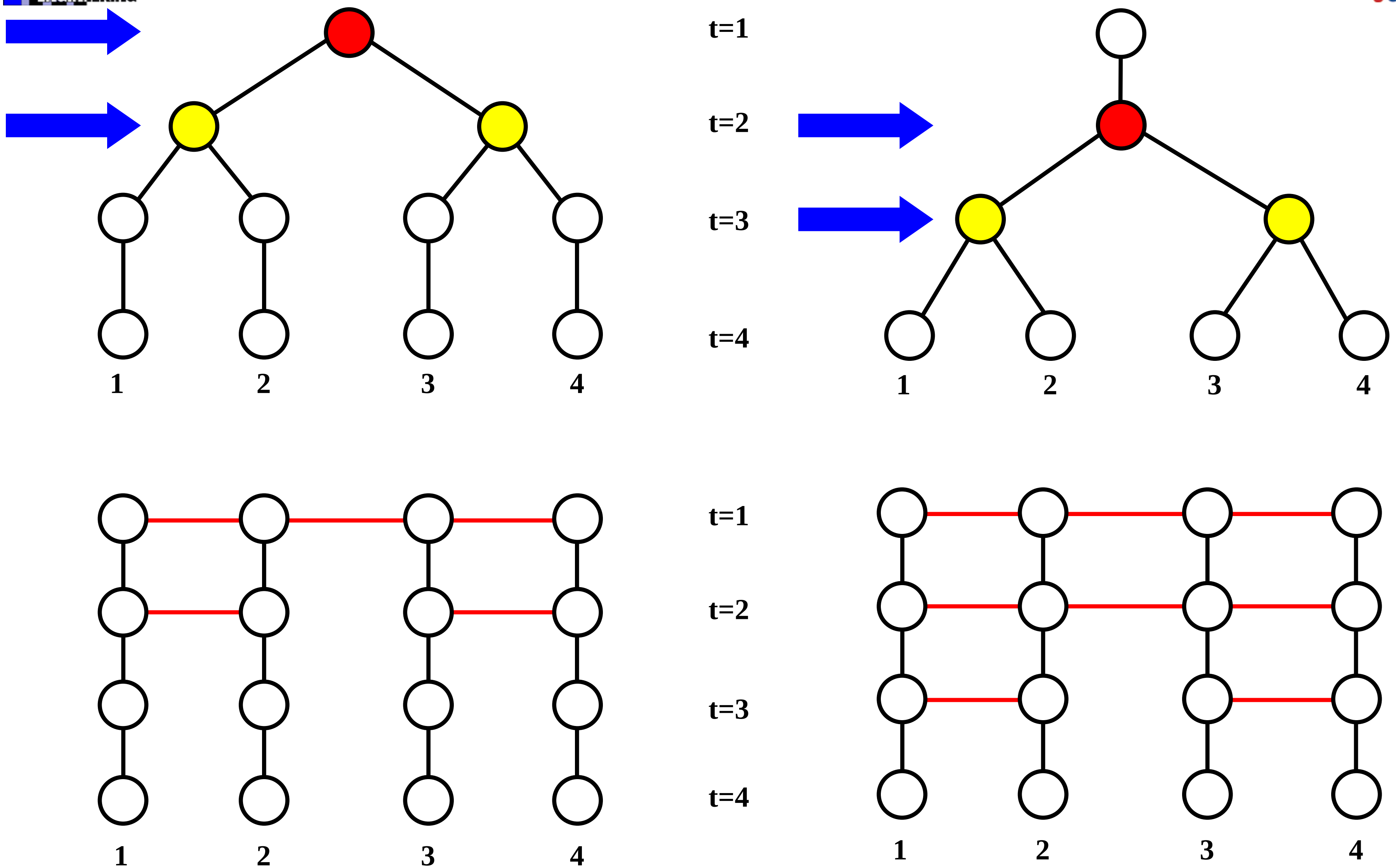


Nodes have same amount of information ≡ Nodes are indistinguishable



Non-anticipativity constraints

Representation of Decision-Dependence Using Scenario Tree



Multi-stage Stochastic Nonconvex MINLP

Maximize.. Probability weighted average of NPV over uncertainty scenarios

subject to

- **Equations about economics of the model**
- **Surface constraints**
- **Non-linear equations related to reservoir performance**
- **Logic constraints relating decisions**

  if there is a TLP available, a TLP well can be drilled

Every scenario, time period

- **Non-anticipativity constraints**

  Non-anticipativity prevents a decision being taken now from using information that will only become available in the future

  Disjunctions (conditional constraints)

Every pair scenarios, time period

Problem size MINLP increases exponentially with number of time periods and scenarios →	**Decomposition algorithm:** ***Lagrangean relaxation & Branch and Bound***

Formulation of Lagrangean dual

Relaxation

- **Relax disjunctions, logic constraints**
- **Penalty for equality constraints**

$^b\lambda_{uf}^{s,s'}, {}^y\lambda^{s,s'}, {}^d\lambda^{s,s'}$: Lagrange Multipliers

$$\text{Max} \quad \sum_s p^s \left[\sum_t \left(c_{1t} q_t^s + c_{2t} d_t^s + c_{3t} y_t^s + \sum_{uf} c_{4t,uf} b_{uf,t}^s \right) \right]$$
$$+ \sum_{(s,s')} \left[\sum_{uf} {}^b\lambda_{uf}^{s,s'} \left(b_{uf,1}^s - b_{uf,1}^{s'} \right) + {}^y\lambda^{s,s'} \left(y_1^s - y_1^{s'} \right) + {}^d\lambda^{s,s'} \left(d_1^s - d_1^{s'} \right) \right]$$

$$\sum_{\tau=1}^{t} \left(A_\tau^s q_\tau^s + B_\tau^s d_\tau^s + C_\tau^s y_\tau^s + \sum_{uf} D_{uf,\tau}^s b_{uf,\tau}^s \right) \le a_t^s \qquad \forall (t,s)$$

Non-anticipativity constraints

$$\begin{bmatrix} & Z_t^{s,s'} & \\ q_t^s & = & q_t^{s'} \\ d_{t+1}^s & = & d_{t+1}^{s'} \\ y_{t+1}^s & = & y_{t+1}^{s'} \\ b_{uf,t+1}^s & = & b_{uf,t+1}^{s'} \quad \forall uf \end{bmatrix} \vee \begin{bmatrix} \neg Z_t^{s,s'} \end{bmatrix} \qquad \forall (t,s,s')$$

$$Z_t^{s,s'} \Leftrightarrow \bigwedge_{uf \in \mathcal{D}(s,s')} \left[\bigwedge_{\tau=1}^{t} \left(\neg b_{uf,\tau}^s \right) \right] \qquad \forall (t,s,s')$$

$$b_{uf,1}^s = b_{uf,1}^{s'} \qquad \forall (uf,s,s')$$
$$d_1^s = d_1^{s'} \qquad \forall (s,s')$$
$$y_1^s = y_1^{s'} \qquad \forall (s,s')$$

One Reservoir Example

Optimize the planning decisions for an oilfield having single reservoir for 10 years.

Decisions:

- **Number, capacity and installation schedule of FPSO/TLP facilities**
- **Number and drilling schedule of sub-sea/TLP wells**
- **Oil production profile over time**

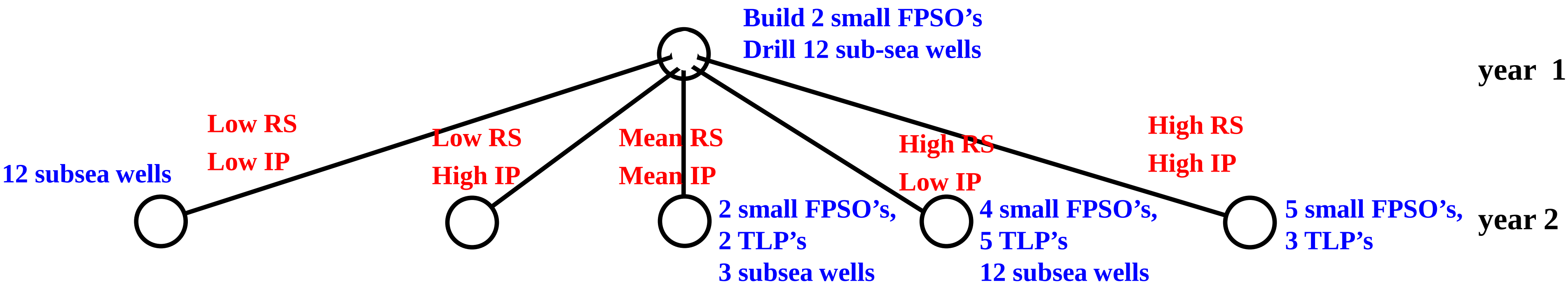
Uncertain Parameters (Discrete Values)	Scenarios							
	1	2	3	4	5	6	7	8
Initial Productivity per well (kbd)	10	10	20	20	10	10	20	20
Reservoir Size (Mbbl)	300	300	300	300	1500	1500	1500	1500
Water Breakthrough Time Parameter	5	2	5	2	5	2	5	2

Construction Lead Time (years)	Wells		Facilities		
	TLP	Sub-sea	TLP	Small FPSO	Large FPSO
	1	1	1	2	4

Multistage Stochastic Programming Approach

RS: Reservoir size
IP: Initial Productivity
BP: Breakthrough Parameter

E[NPV] = $4.92 x 10⁹

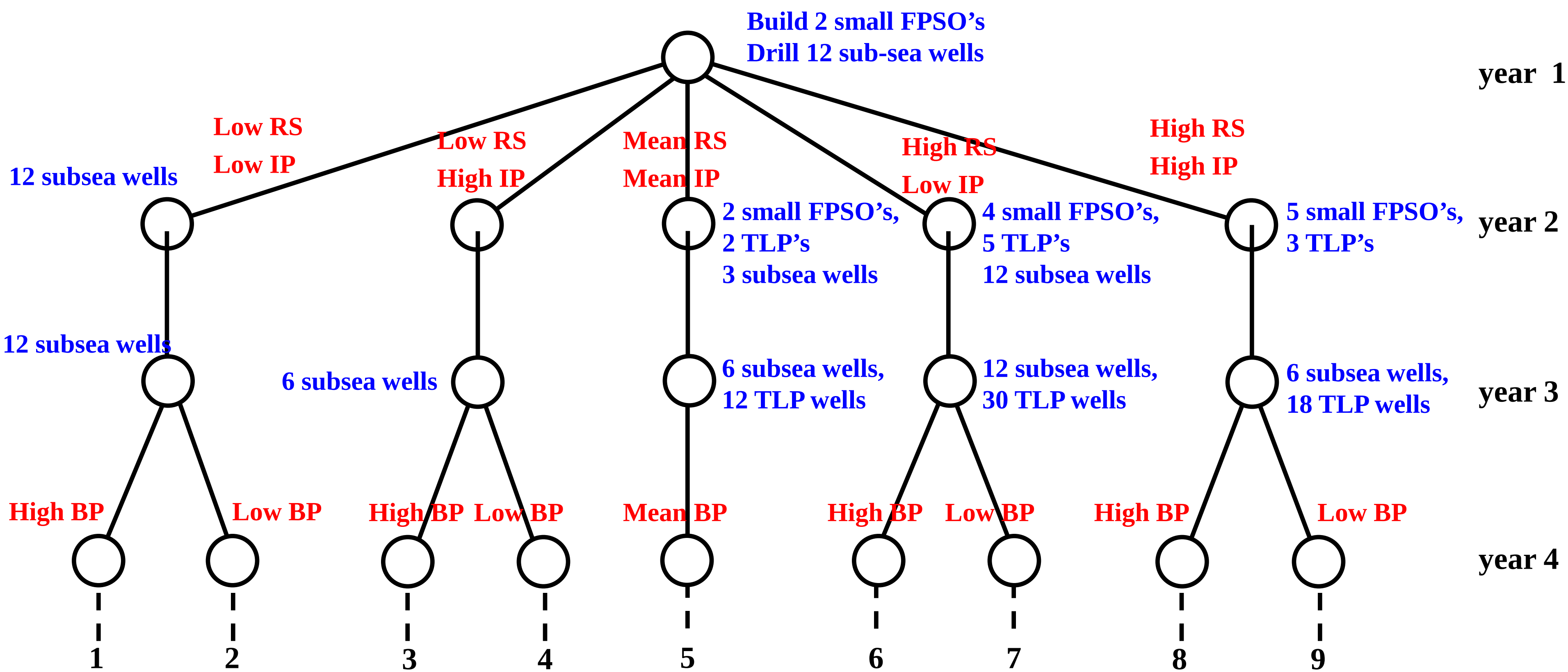


Solution proposes building 2 small FPSO's in the first year and then add new facilities / drill wells (recourse action) depending on the positive or negative outcomes.

Multistage Stochastic Programming Approach

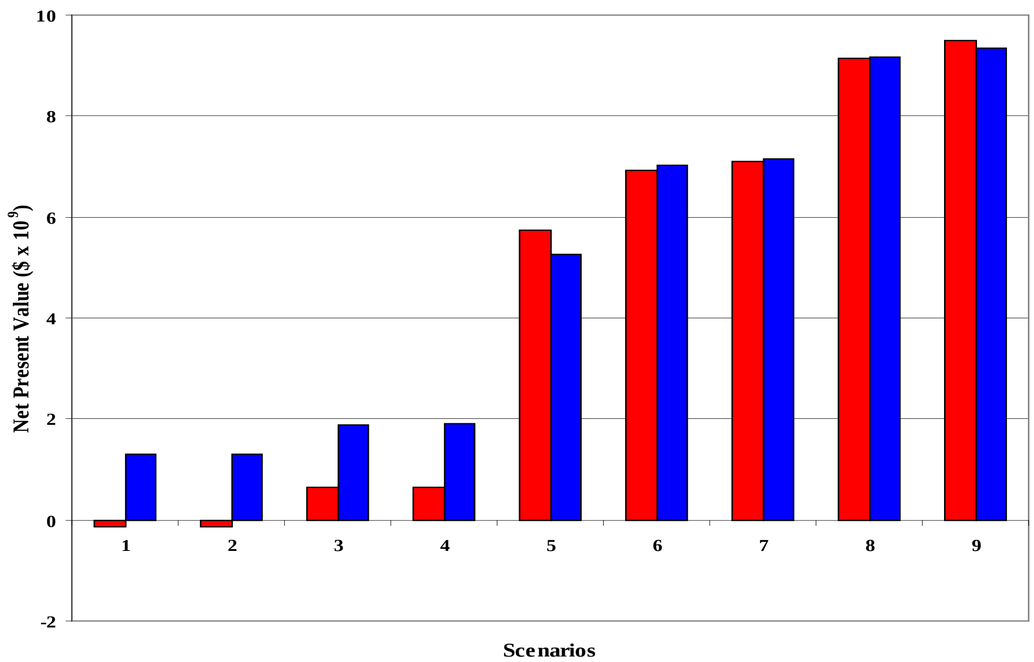
RS: Reservoir size
IP: Initial Productivity
BP: Breakthrough Parameter

E[NPV] = $4.92 x 10^9



Solution proposes building 2 small FPSO's in the first year and then add new facilities / drill wells (recourse action) depending on the positive or negative outcomes.

Distribution of Net Present Value



Deterministic Mean Value = $4.38 x 10^9$

Multistage Stoch Progr = $4.92 x 10^9$ ***=> 12% higher and more robust***

Computation: Algorithm 1: 120 hrs; Algorithm 2: 5.2 hrs
Nonconvex MINLP: 1400 discrete vars, 970 cont vars, 8090 Constraints

Economics vs. performance?

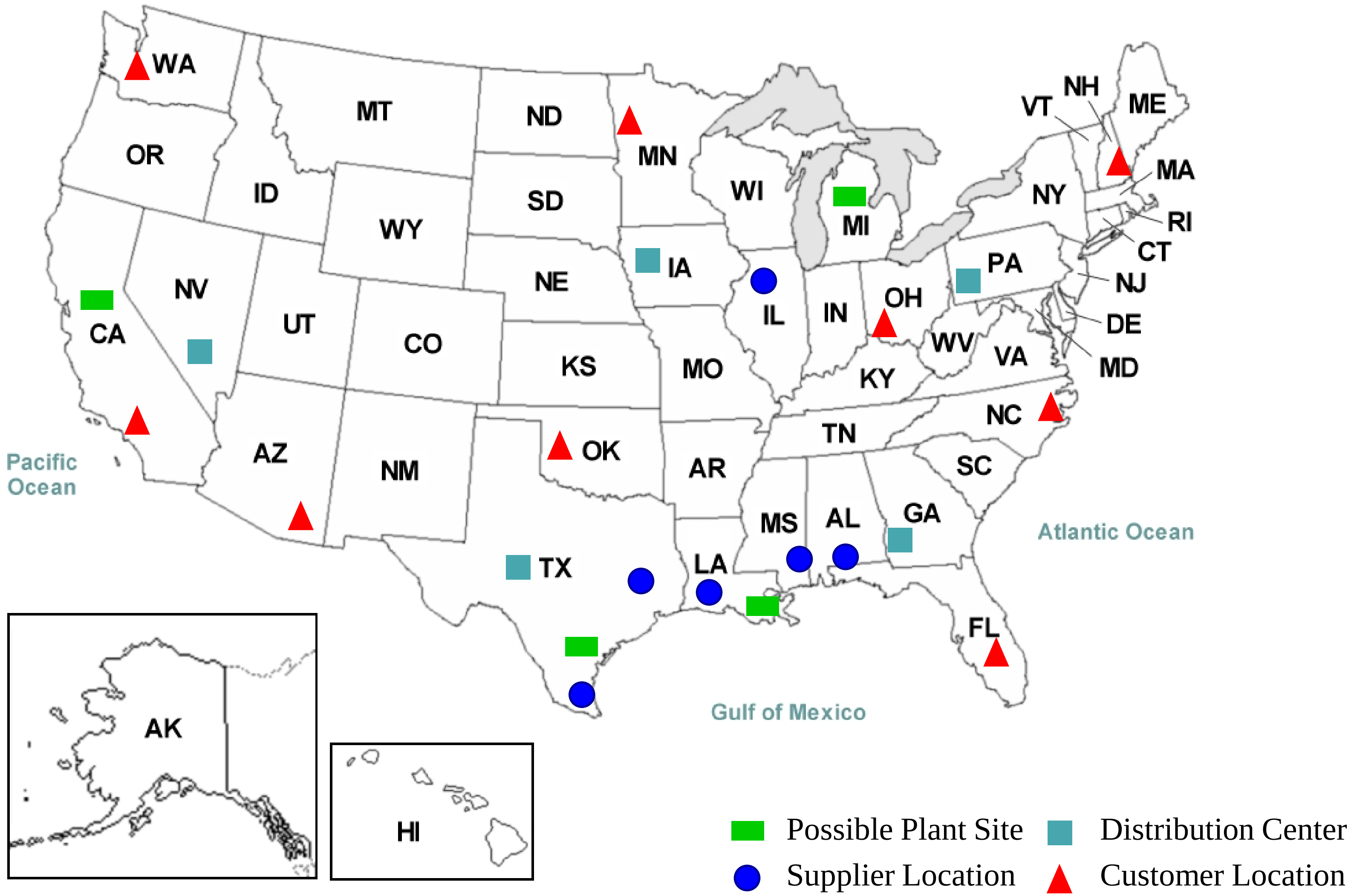
Multiobjective Optimization Approach

Economics vs Environmental:
Guillen-Gozalbez, Grossmann (2010)
Pinto-Varela, Barbosa-Póvoa and A.Q. Novais (2011)

Optimal Design of Responsive Process Supply Chains

Objective: design supply chain polystyrene resisns under responsive and economic criteria

You, Grossmann (2008)



Carnegie Mellon

Production Network of Polystyrene Resins

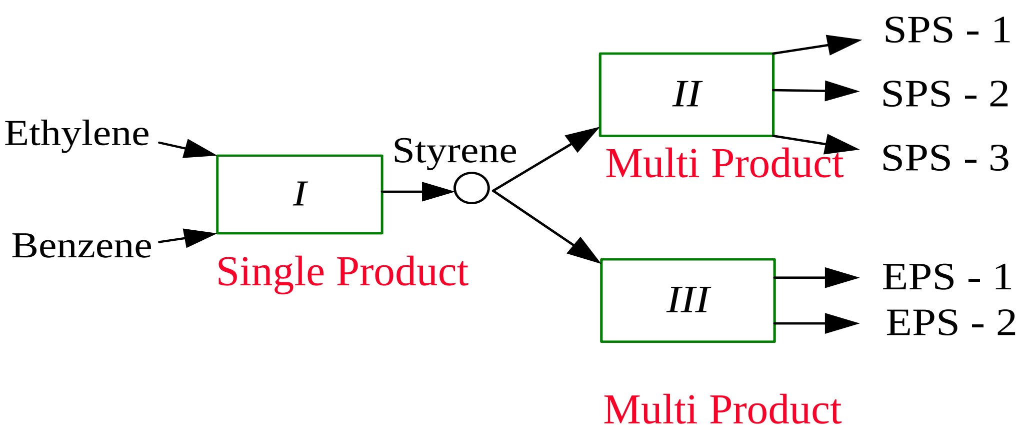
Three types of plants:

Plant *I*: *Ethylene + Benzene* ⟶ *Styrene* (1 products)

Plant *II*: *Styrene* ⟶ *Solid Polystyrene (SPS)* (3 products)

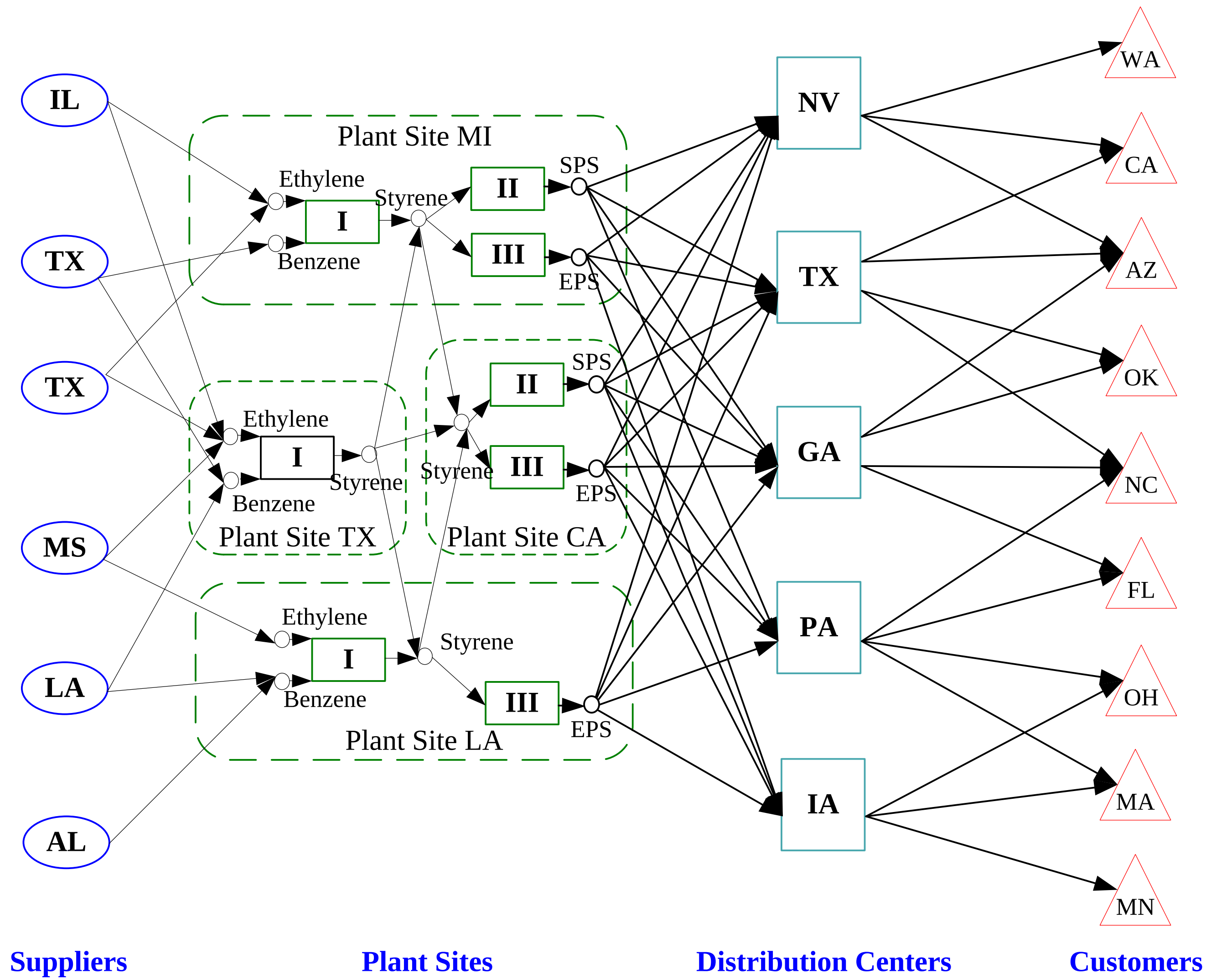
Plant *III*: *Styrene* ⟶ *Expandable Polystyrene (EPS)* (2 products)

Basic Production Network



Source: Data Courtesy Nova Chemical Inc. http://www.novachem.com/

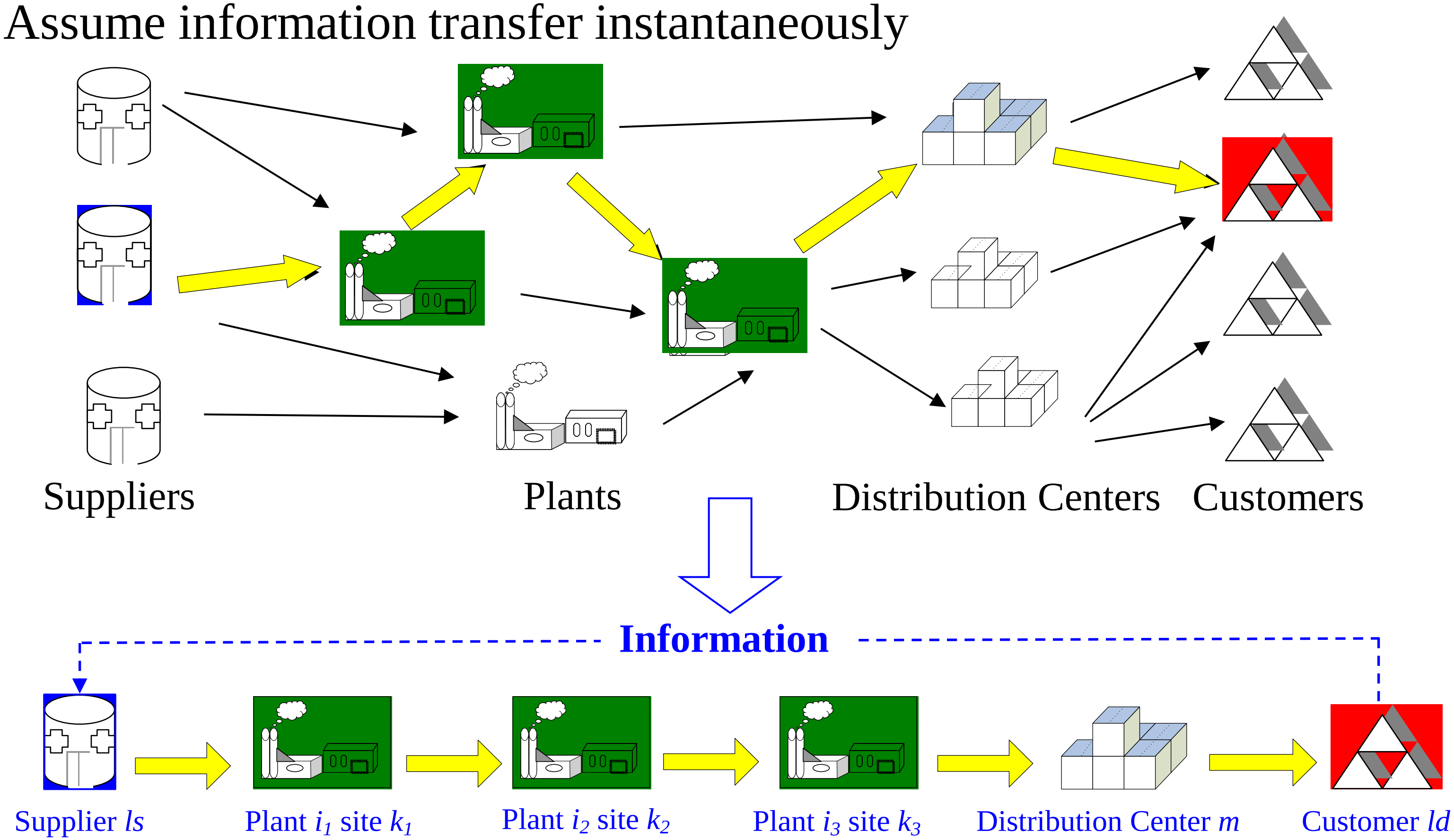
Potential Network Superstructure



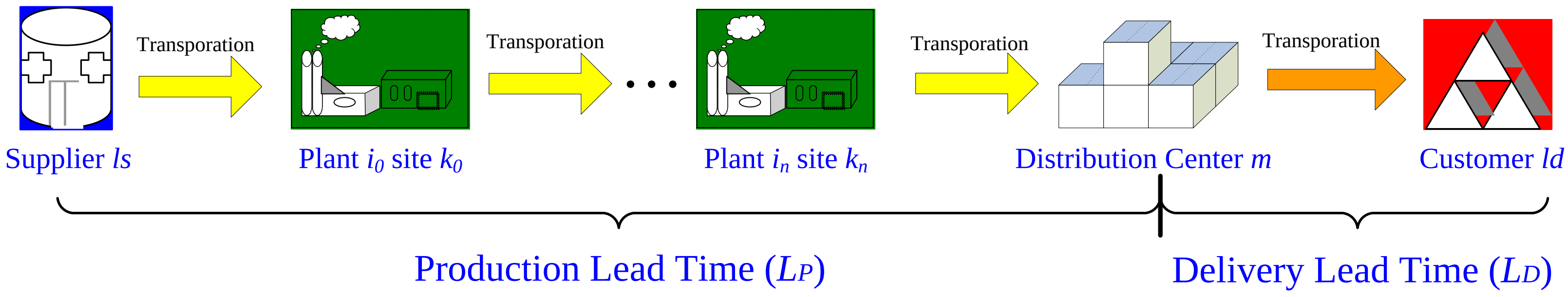
Responsiveness - Lead Time

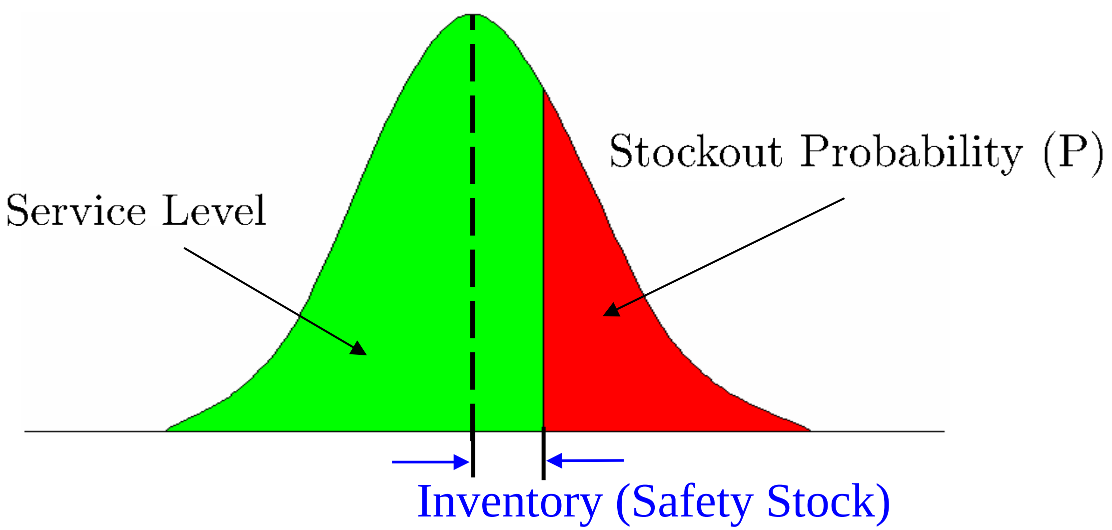
Lead Time for A Linear Supply Chain

- A supply chain network = ∑Linear supply chains
  - Assume information transfer instantaneously



Lead Time under Demand Uncertainty





$$\text{Expected Lead Time} = L_D + \text{P(Stockout)} \cdot L_P$$

Bi-criterion Multiperiod MINLP Formulation

Choose Discrete (0-1), continuous variables

- Objective Function:
  - Max: Net Present Value
  - Min: Expected Lead time

  } Bi-criterion

- Constraints:
  - Network structure constraints

Suppliers – plant sites Relationship

Plant sites – Distribution Center

Input and output relationship of a plant

Distribution Center – Customers

Cost constraint

  - Operation planning constraints

Production constraint

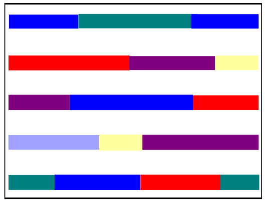
Capacity constraint

Mass balance constraint

Demand constraint

Upper bound constraint

  - Cyclic scheduling constraints



Assignment constraint

Sequence constraint

Demand constraint

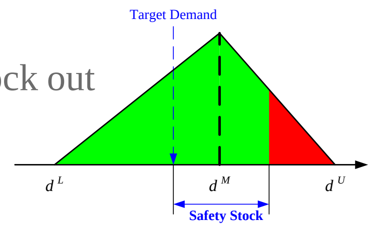
Production constraint

Cost constraint

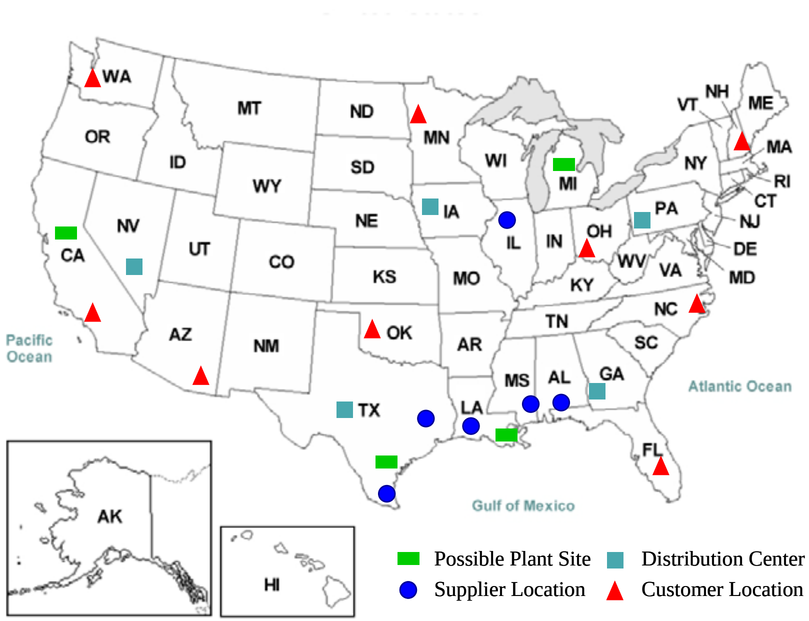
  - Probabilistic constraints

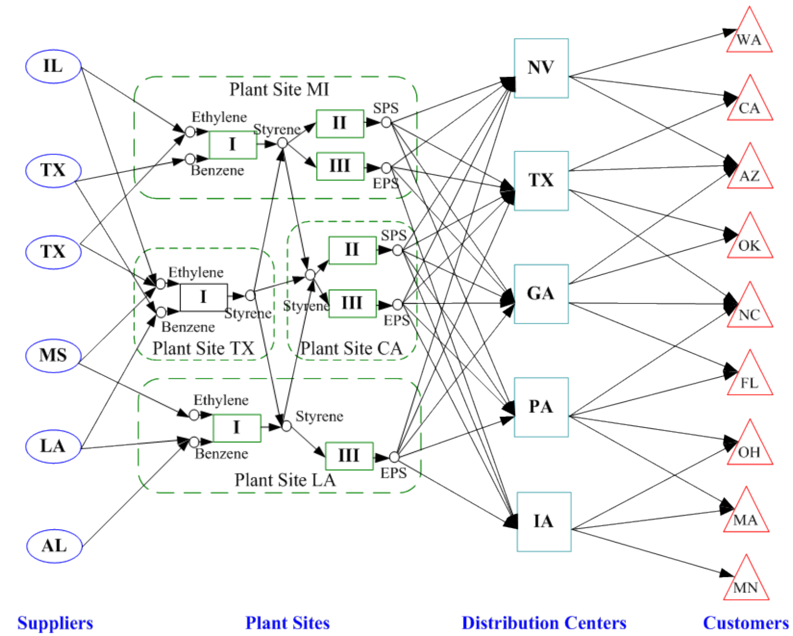
Chance constraint for stock out

(reformulations)



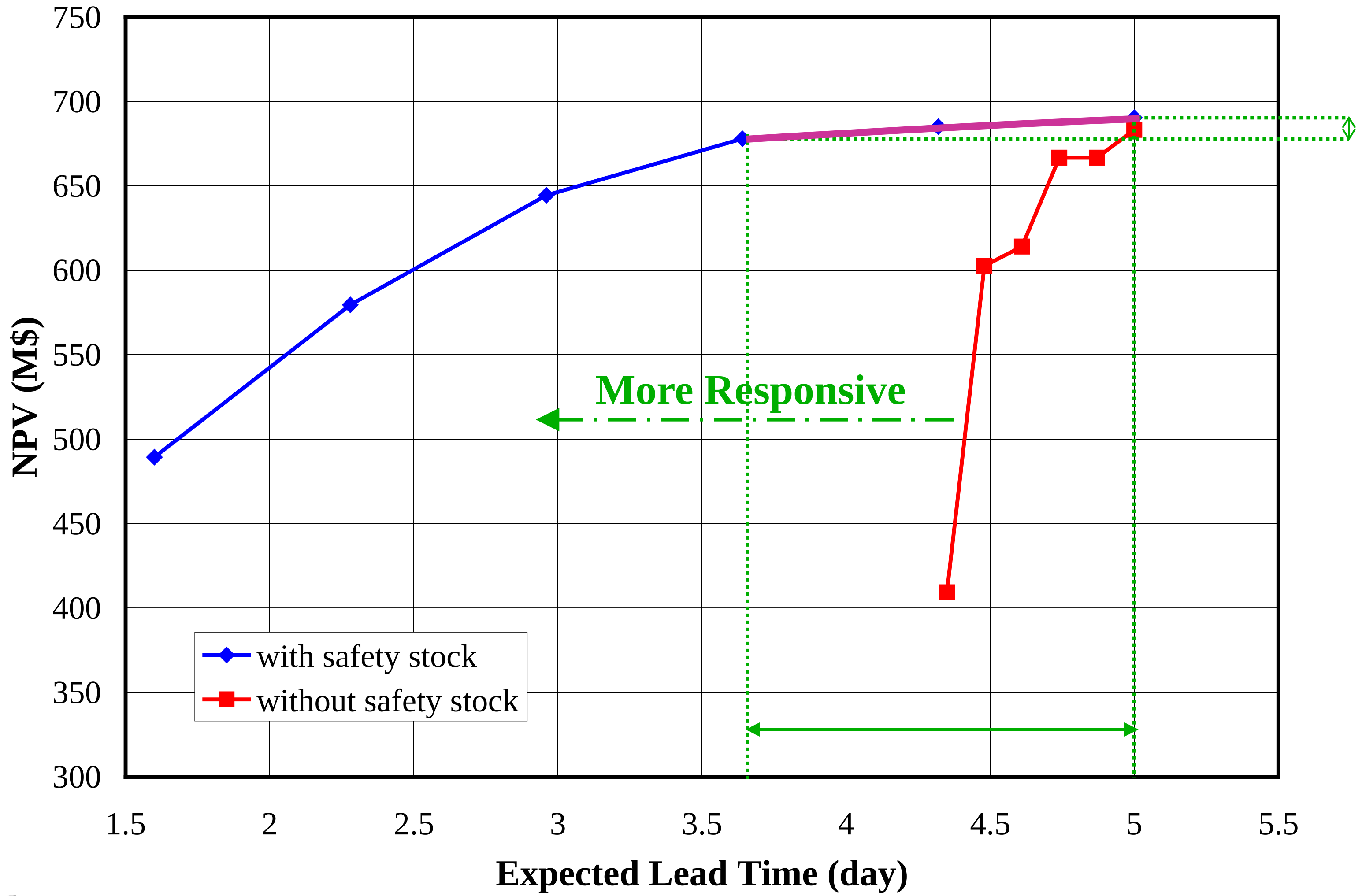
Case Study





- Problem Size:
  - # of Discrete Variables: 215
  - # of Continuous Variables: 8126
  - # of Constraints: 14617
- Solution Time:
  - Solver: GAMS/BARON
  - Direct Solution: > 2 weeks
  - Proposed Algorithm: ~ 4 hours

Pareto Curves – with and without safety stock



Chemical Engineering
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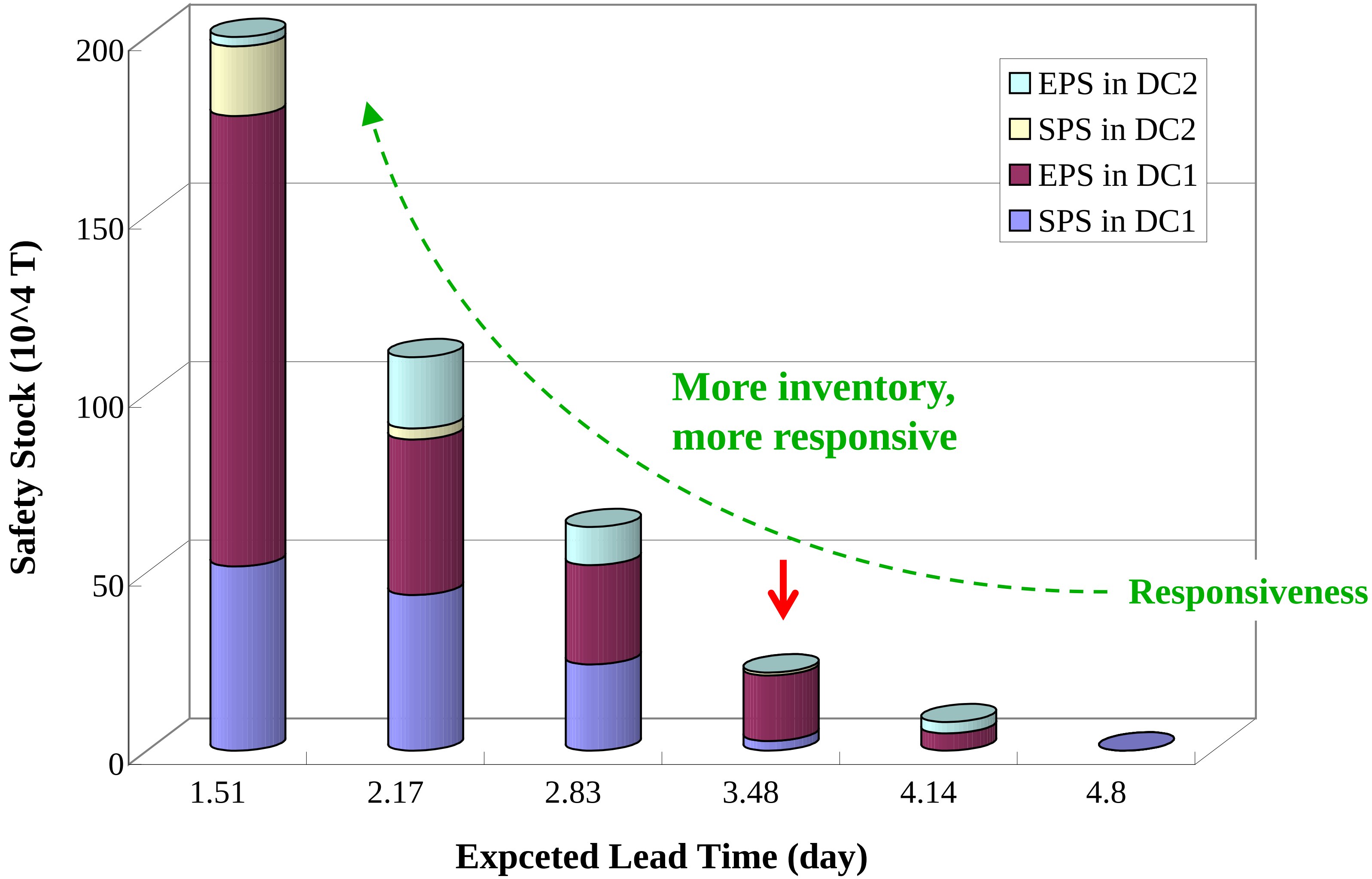
Safety Stock Levels - Expected Lead Time



Other Issues / Future Directions

1. Integration of control with planning and scheduling

Bhatia, Biegler (1996), Perea, Ydstie, Grossmann (2003), Flores, Grossmann (2006), Prata, Oldenburg, Kroll, Marquardt (2008) , Harjunkoski, Nystrom, Horch (2009)

Challenge: Effective solution of Mixed-Integer Dynamic Optimization (MIDO)

2. Optimization of entire supply chains

Challenges:

- **Combining different models (eg maritime and vehicle transportation, pipelines)**
  Cafaro, Cerda (2004), Relvas, Matos, Barbosa-Póvoa, Fialho, Pinheiro (2006)
- **Advanced financial models**
  Van den Heever, Grossmann (2000), Guillén, Badell, Espuña, Puigjaner (2006),

3. Design and Operation of Sustainable Supply Chains

Challenges:

Biofuels, Energy, Environmental

Elia, Baliban, Floudas (2011) Guillén-Gosálbez (2011), You, Tao, Graziano, Snyder (2011)

Conclusions

1. **Enterprise-wide Optimization area of great industrial interest**

   Great economic impact for effectively managing complex supply chains

2. **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)