Advances in Mathematical Programming Models for Enterprise-wide Optimization

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Motivation for Enterprise-wide Optimization

US chemical industry:

19 % of the world's chemical output
US$689 billion revenues
10% of US exports

Facing stronger international competition
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)

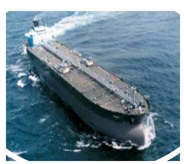
EWO involves optimizing the operations of R&D, material supply, manufacturing, distribution of a company to reduce costs, inventories, ecological footprint and to maximize profits, responsiveness .

Key element: Supply Chain

Example: petroleum industry

Wellhead

Trading

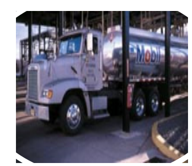


Transfer of Crude

Refinery Processing

Schedule Products

Transfer of Products



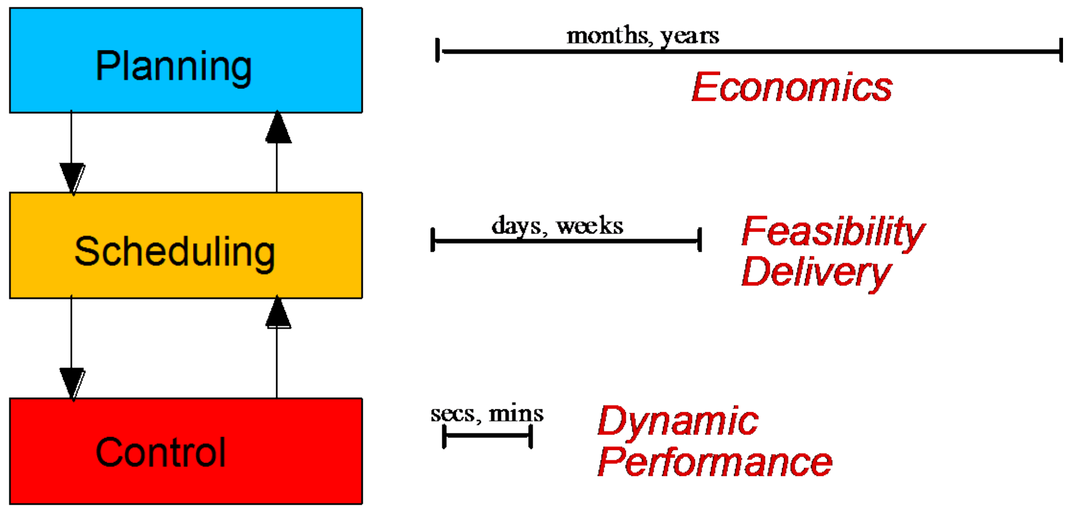
Terminal Loading

Pump

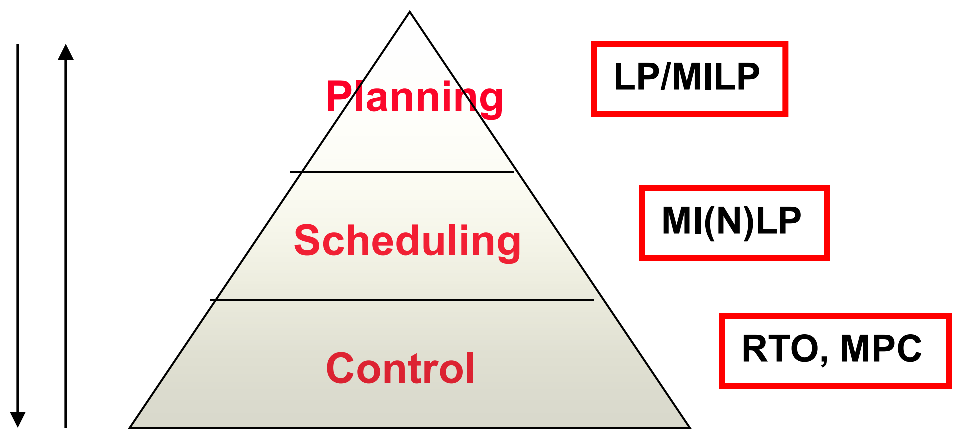
Key issues:

I. Integration of planning, scheduling and control

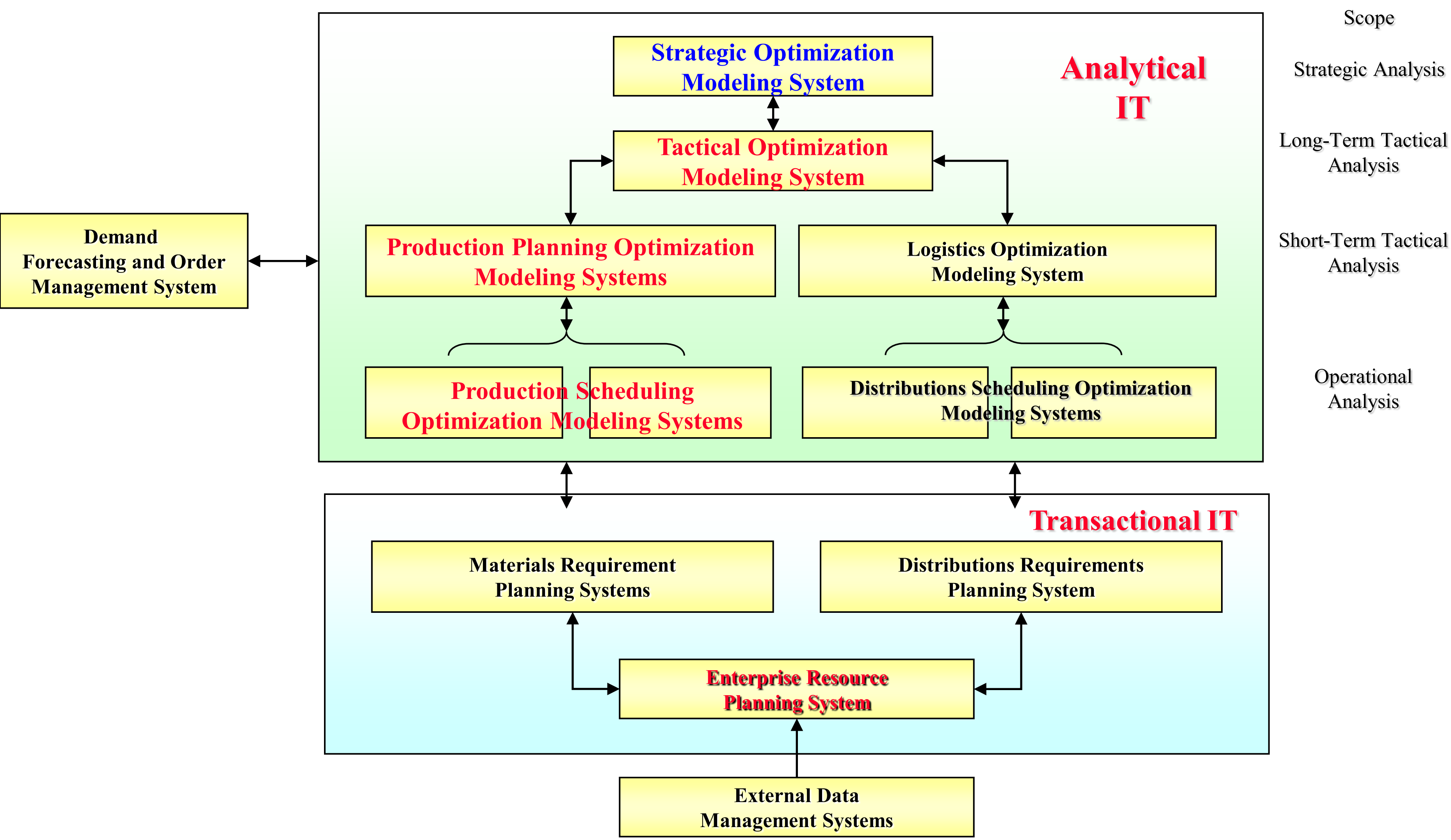
Mutiple time scales



Mutiple models



II. Integration of information and models/solution methods



Source: Tayur, et al. [1999]

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Optimization Modeling Framework: Mathematical Programming

$$\min Z = f(x, y)$$ Objective function

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

$$g(x, y) \leq 0$$ 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)* } Global Optimization
Couenne *Belotti, Margot (2008)* }

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

Issues:
Convergence
Nonconvexities

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

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

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 Peterssson (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)* } Global Optimization
Couenne *Belotti, Margot (2008)* } 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*)

Other logic-based: *Constraint Programming (Hooker, 2000)*

Codes: *CHIP, Eclipse, ILOG-CP*

Multistage Stochastic Programming

Birge & Louveaux, 1997; Sahinidis, 2004

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

s.t.

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

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

$$\vdots$$

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

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

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)

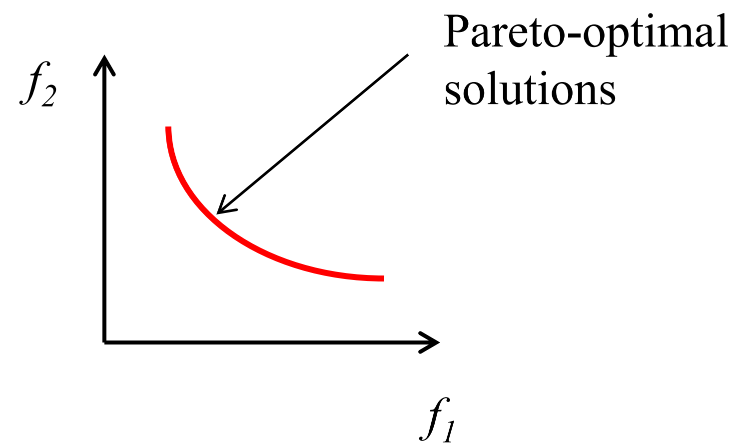
Multiobjective Optimization

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

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

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

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



ε-constraint method:* *Ehrgott (2000)

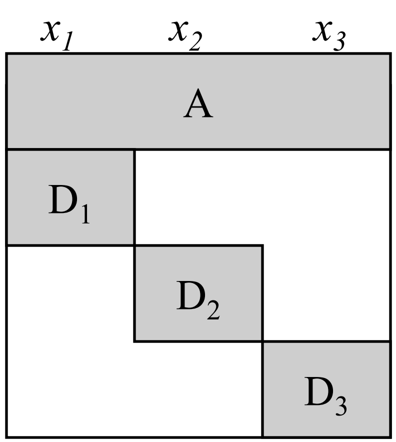
Parametric programming:* *Pistikopoulos, Georgiadis and Dua (2007)

Decomposition Techniques

Lagrangean decomposition

Geoffrion (1972) Guinard (2003)

Complicating Constraints



complicating constraints → $st \; Ax = b$

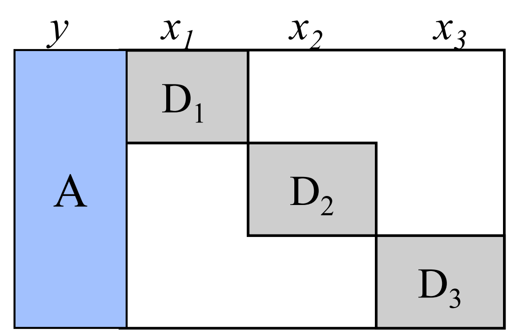
$$\max \; c^T x$$
$$st \;\; Ax = b$$
$$D_i x_i = d_i \;\; i = 1,..n$$
$$x \in X = \{x \,|\, x_i \,, i = 1,..n, |\, x_i \geq 0\}$$

Widely used in EWO

Benders decomposition

Benders (1962), Magnanti, Wing (1984)

Complicating Variables



complicating variables → Ay

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

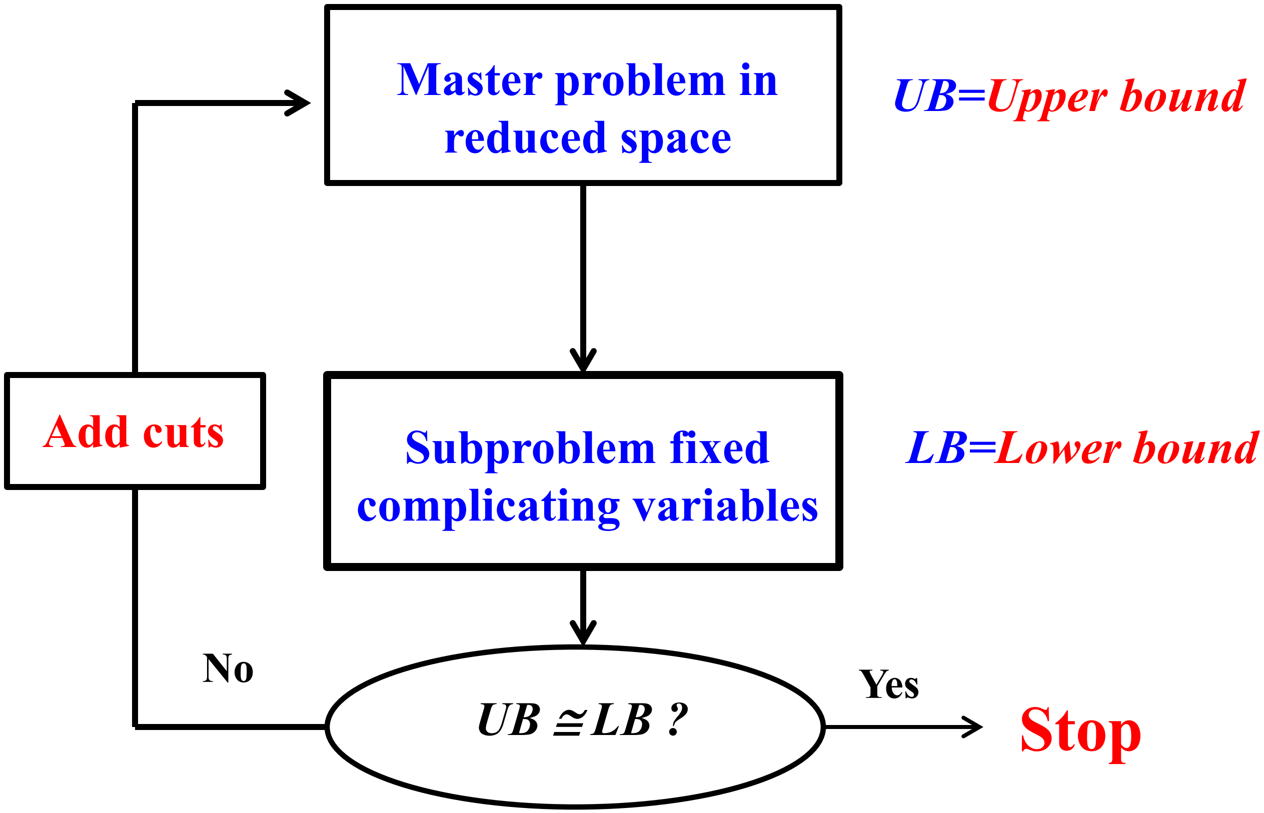
Applied in 2-stage Stochastic Programming

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"

CAPD CENTER

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*

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

Air Products: Design of Resilient Supply Chain Networks for Chemicals and Gases
Contact: James Hutton — *Larry Snyder, Katya Scheinberg*

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

Cognizant: Optimization of gas pipelines
Contact: Phani Sistu — *Larry Biegler, Ajit Gopalakrishnan*

Dow: Multisite Planning and Scheduling Multiproduct Batch Processes
Contact: John Wassick — *Ignacio Grossmann, Bruno Calfa*

Dow: Batch Scheduling and Dynamic Optimization
Contact: John Wassick — *Larry Biegler, Yisu Nie*

Ecopetrol: Nonlinear programming for refinery optimization
Contact: Sandra Milena Montagut — *Larry Biegler, Yi-dong Lang*

ExxonMobil: Global optimization of multiperiod blending networks
Contact: Shiva Kameswaran, Kevin Furman — *Ignacio Grossmann, Scott Kolodziej*

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

G&S Construction: Modeling & Optimization of Advanced Power Plants
Contact: Daeho Ko and Dongha Lim — *Larry Biegler, Yi-dong Lang*

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

UNILEVER: Scheduling of ice cream production
Contact: Peter Bongers — *Ignacio Grossmann, Martijn van Elzakker*

BP: Refinery Planning with Process Models*
Contact: Ignasi Palou-Rivera — *Ignacio Grossmann, Abdul Alattas*

PPG: Planning and Scheduling for Glass Production*
Contact: Jiao Yu — *Ignacio Grossmann, Ricardo Lima*

TOTAL: Scheduling of crude oil operations*
Contact: Pierre Pestiaux — *Ignacio Grossmann, Sylvain Mouret*

Major Issues

-Linear vs Nonlinear models

- The multi-scale optimization challenge

- The uncertainty challenge

- Economics vs performance

- Computational efficiency in large-scale problems

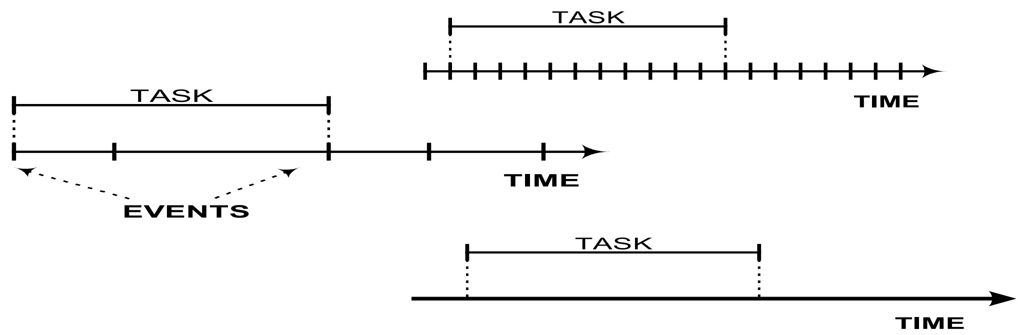
- Commercial vs. Off-the Shelf Software

Why Emphasis on Linear?

Rich developments in Batch Scheduling dominated by MILP

(A) Time Domain Representation

- Discrete time
- Continuous time



(B) Event Representation

Discrete Time

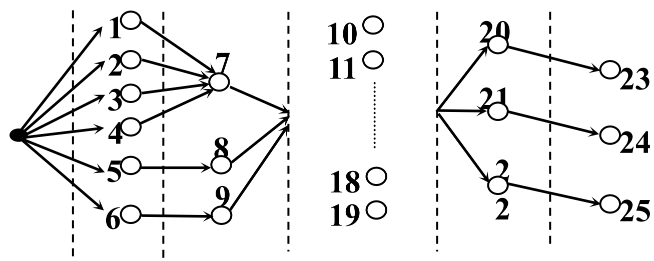
- Global time intervals

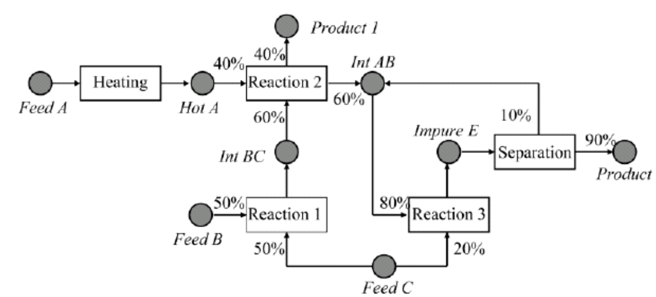
Continuous Time

- Time slots, Unit-specific direct precedence, Global direct or general precedence, Global time points Unit- specific time event

(C) Plant topology

- Multistage
- Network (STN,RTN)





(D) Objective Functions: Makespan, Earliness/ Tardiness, Profit, Inventory, Cost

Pioneers: *Rekalitis, Rippin: late 1970's*

Most cited paper: *Kondili, Pantelides, Sargent (1993) MILP-STN Paper: 460 citations (Web Science)*

Reviews: *Lin, Floudas (2004), Mendez, Cerdá , Grossmann, Harjunkoski (2006)*

Unification and Generalization: *Sundaramoorthy, Maravelias (2011)*

-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%)

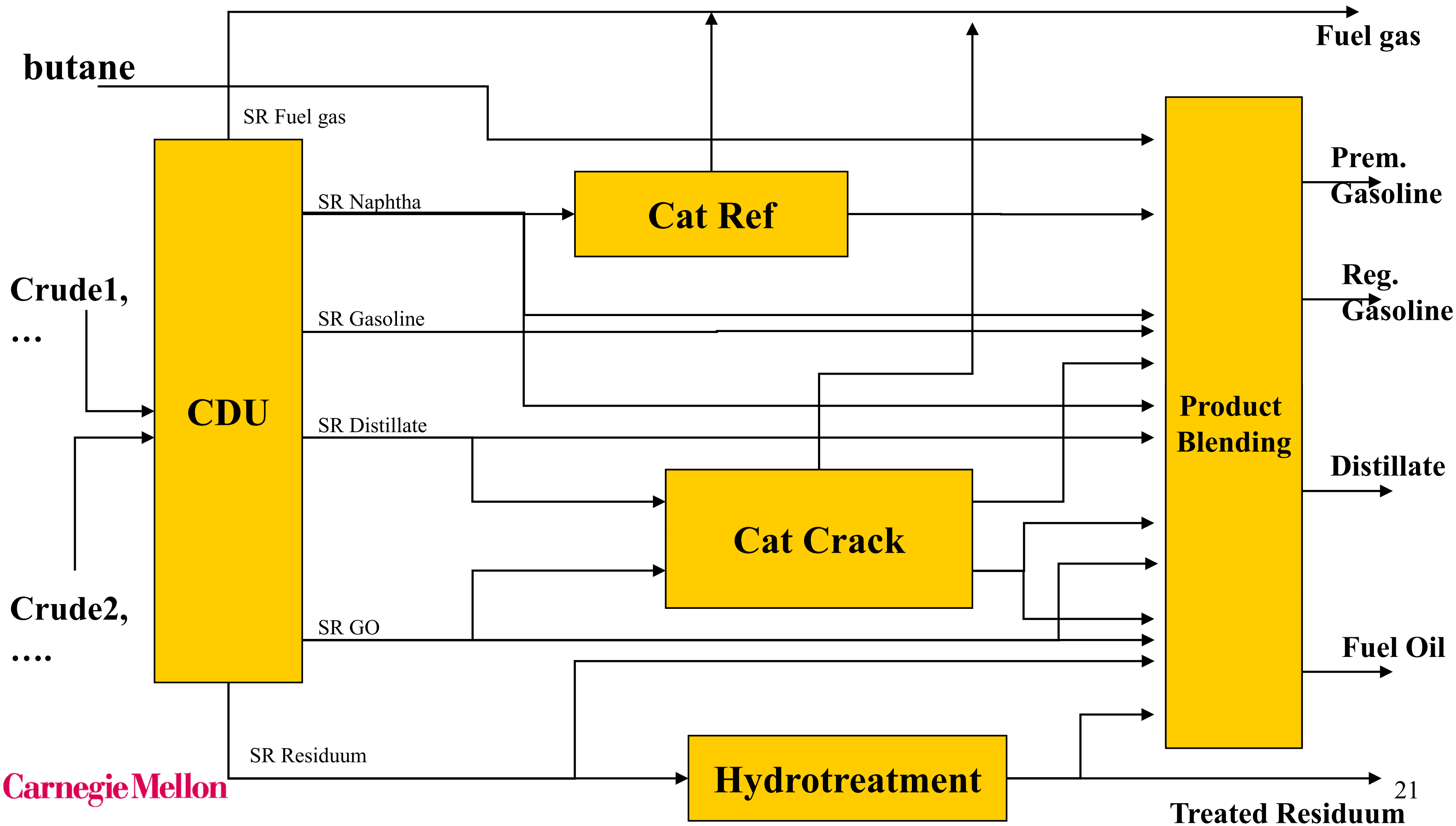
CPU-time: 27 secs!!!

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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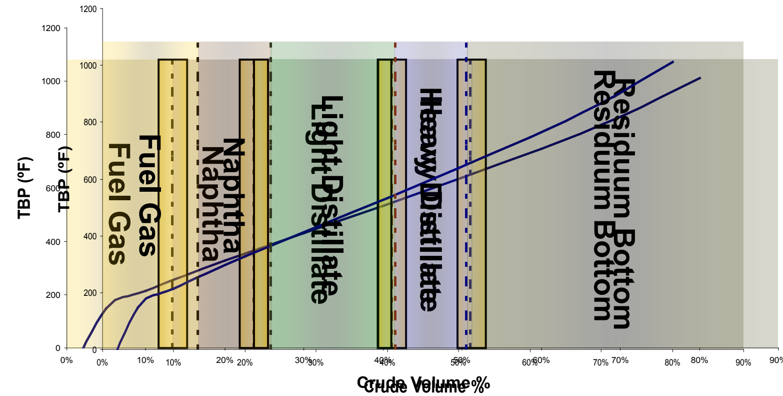
Refinery Planning Models

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
3 Crude Oil Case	*FY*	159	185		**0.250**	CPLEX
	SC	174	215		**0.281**	
	FI	1770	1808	522	**0.439**	CONOPT
4 Crude Oil Case	*FY*	192	231		**0.218**	CPLEX
	SC	212	271		**0.241**	
	FI	2340	2395	696	**0.860**	CONOPT

-   Solution large-scale problems:

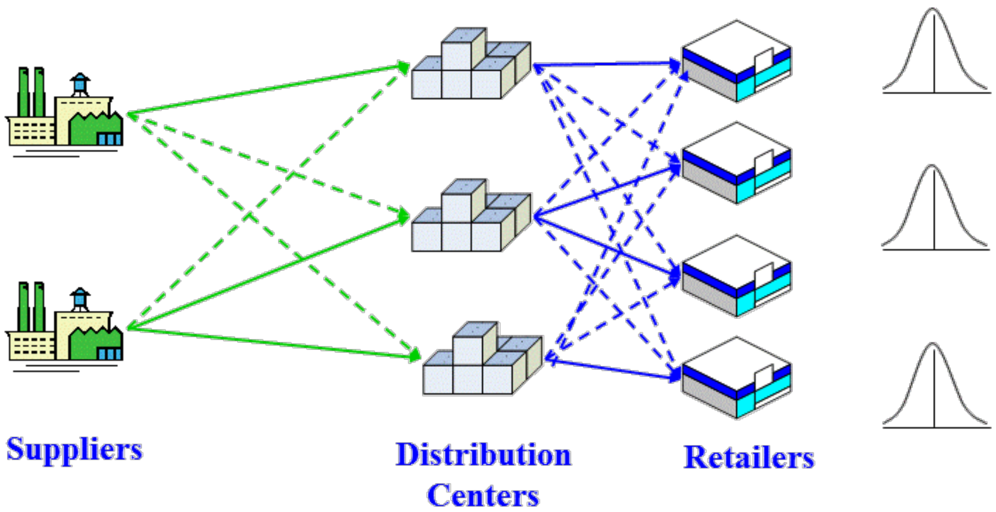
Strategy 1: Exploit problem structure (TSP)

Strategy 2: Decomposition

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

Design Supply Chain Stochastic Inventory

You, Grossmann (2008)

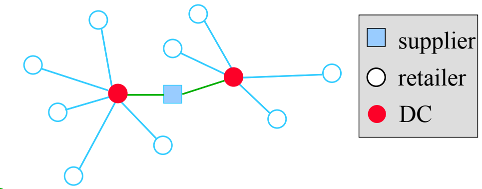


- Major Decisions (Network + Inventory)
  - Network: number of DCs and their locations, assignments between retailers and DCs (single sourcing), shipping amounts
  - Inventory: number of replenishment, reorder point, order quantity, safety stock

- 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



$$\min \quad \sum_{j \in J} f_j X_j$$ 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

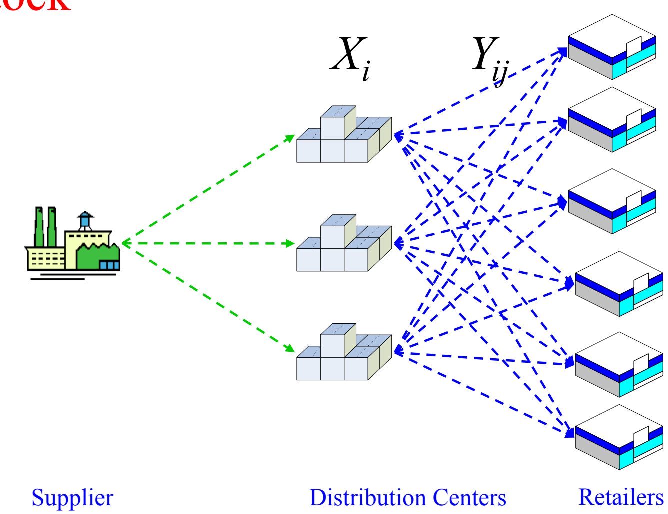
$$+ \sum_{j \in J} \left(\theta h z_\alpha \sqrt{\sum_{i \in I} \sigma_i^2 L_i Y_{ij}}\right)$$ Safety Stock

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

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

(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)**

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						BARON (global optimum)		
				Upper Bound	Lower Bound	Gap	Iter.	Time (s)		Upper Bound	Lower Bound	Gap
88	0.001	0.1		867.55	867.54	**0.001 %**	21	**356.1**		867.55	837.68	3.566 %
88	0.001	0.5		1230.99	1223.46	**0.615 %**	24	**322.54**		1295.02*	1165.15	11.146 %
88	0.005	0.1		2284.06	2280.74	**0.146 %**	55	**840.28**		2297.80*	2075.51	10.710 %
88	0.005	0.5		2918.3	2903.38	**0.514 %**	51	**934.85**		3022.67*	2417.06	25.056 %
150	0.001	0.5		1847.93	1847.25	**0.037 %**	13	**659.1**		1847.93	1674.08	10.385 %
150	0.005	0.1		3689.71	3648.4	**1.132 %**	53	**3061.2**		3689.71	3290.18	12.143 %

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

The multi-scale optimization challenge

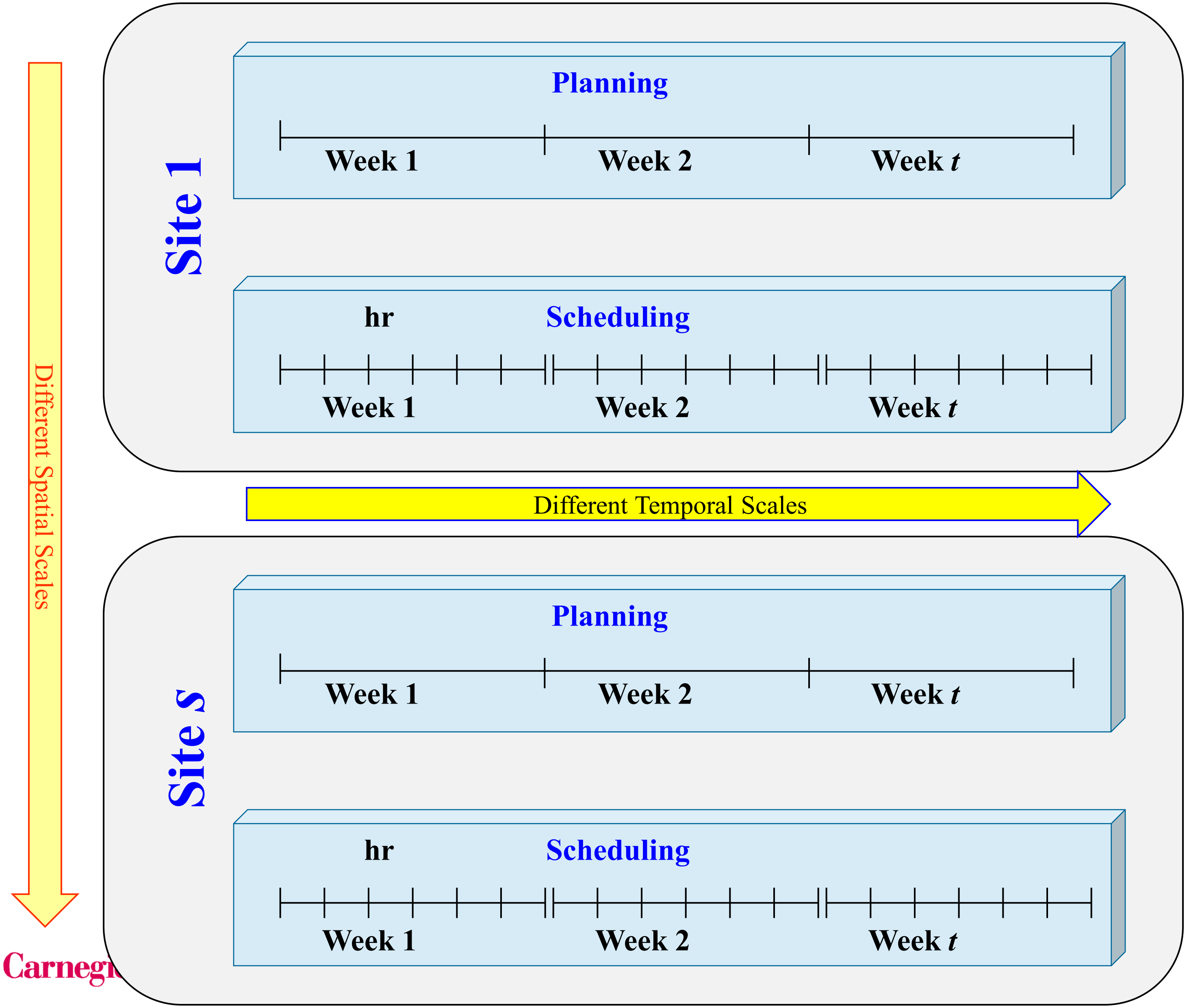
Temporal integration long-term, medium-term and short-term *Bassett, Pekny, Reklaitis (1993), Gupta, Maranas (1999), Jackson, Grossmann (2003), Stefansson, Shah, Jenssen (2006), Erdirik-Dogan, Grossmann (2006), Maravelias, Sung (2009), Li and Ierapetritou (2009), Verderame , Floudas (2010)*

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)

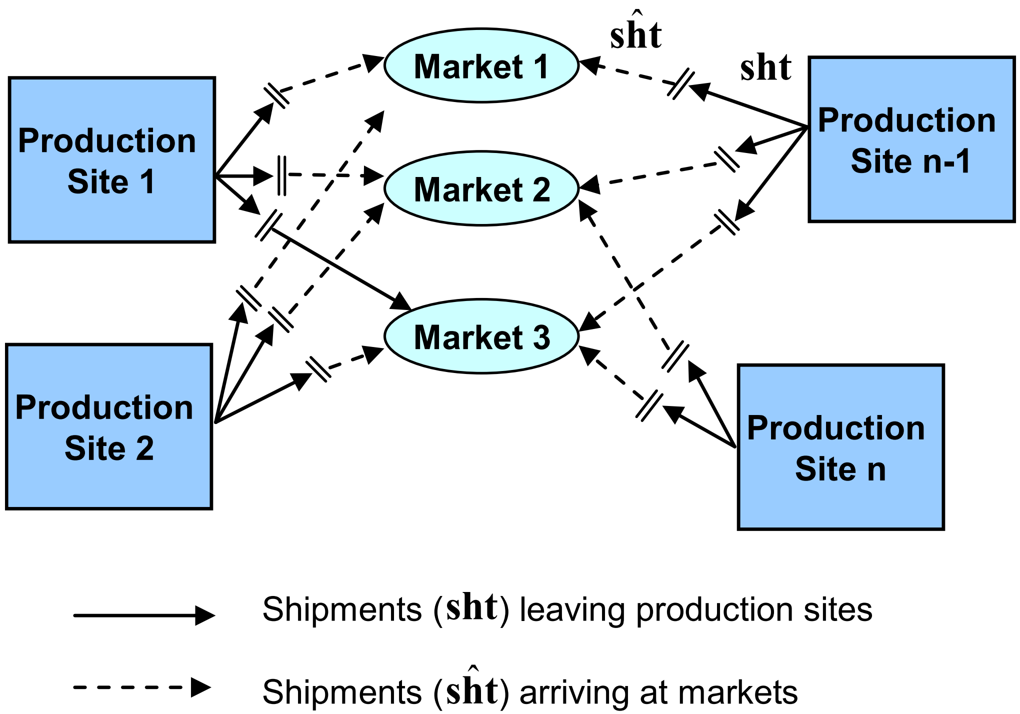
Detailed operation

- Start and end times
- Allocation to parallel lines

Weekly aggregate production:

Detailed operation

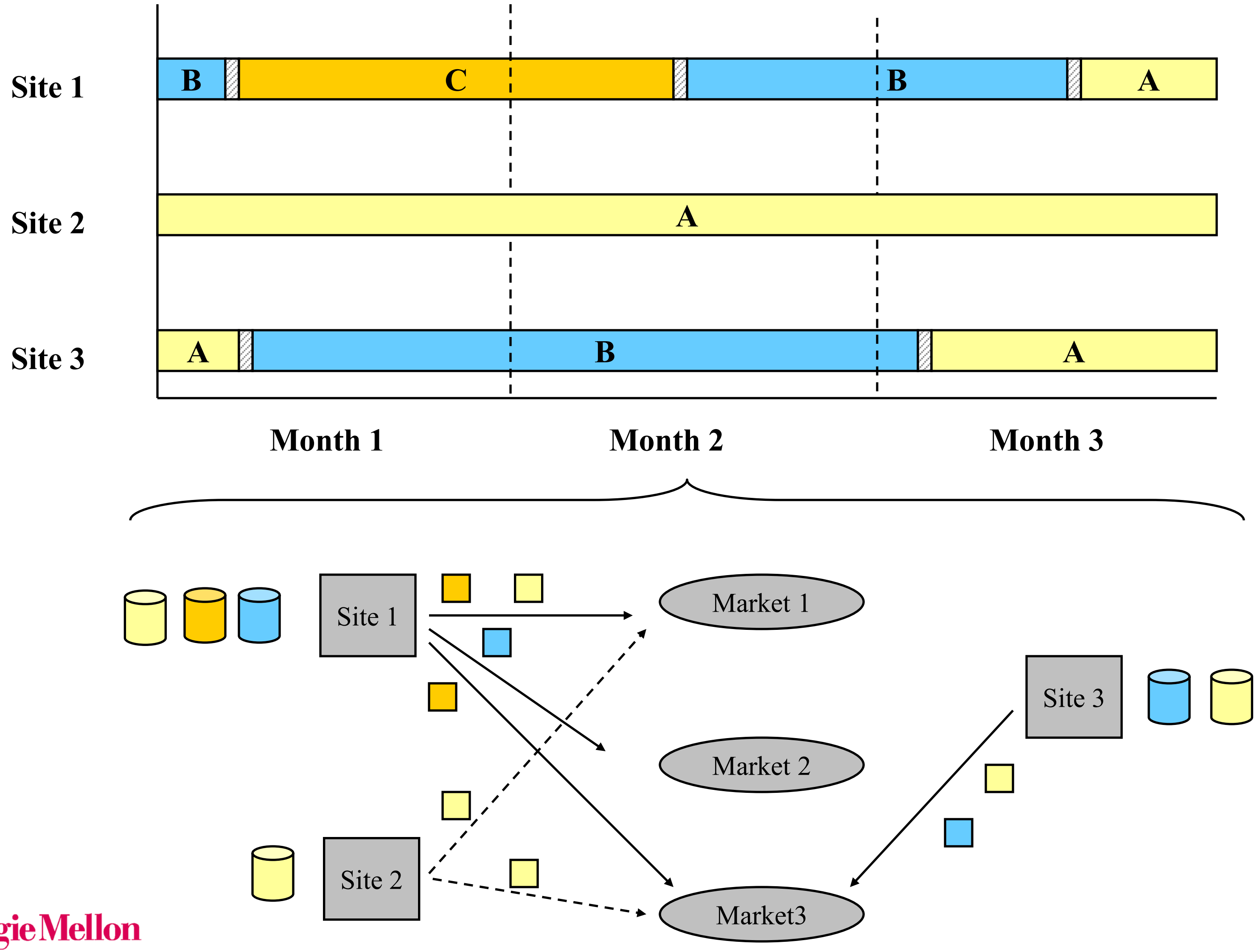
Bilevel decomposition + Lagrangean decomposition



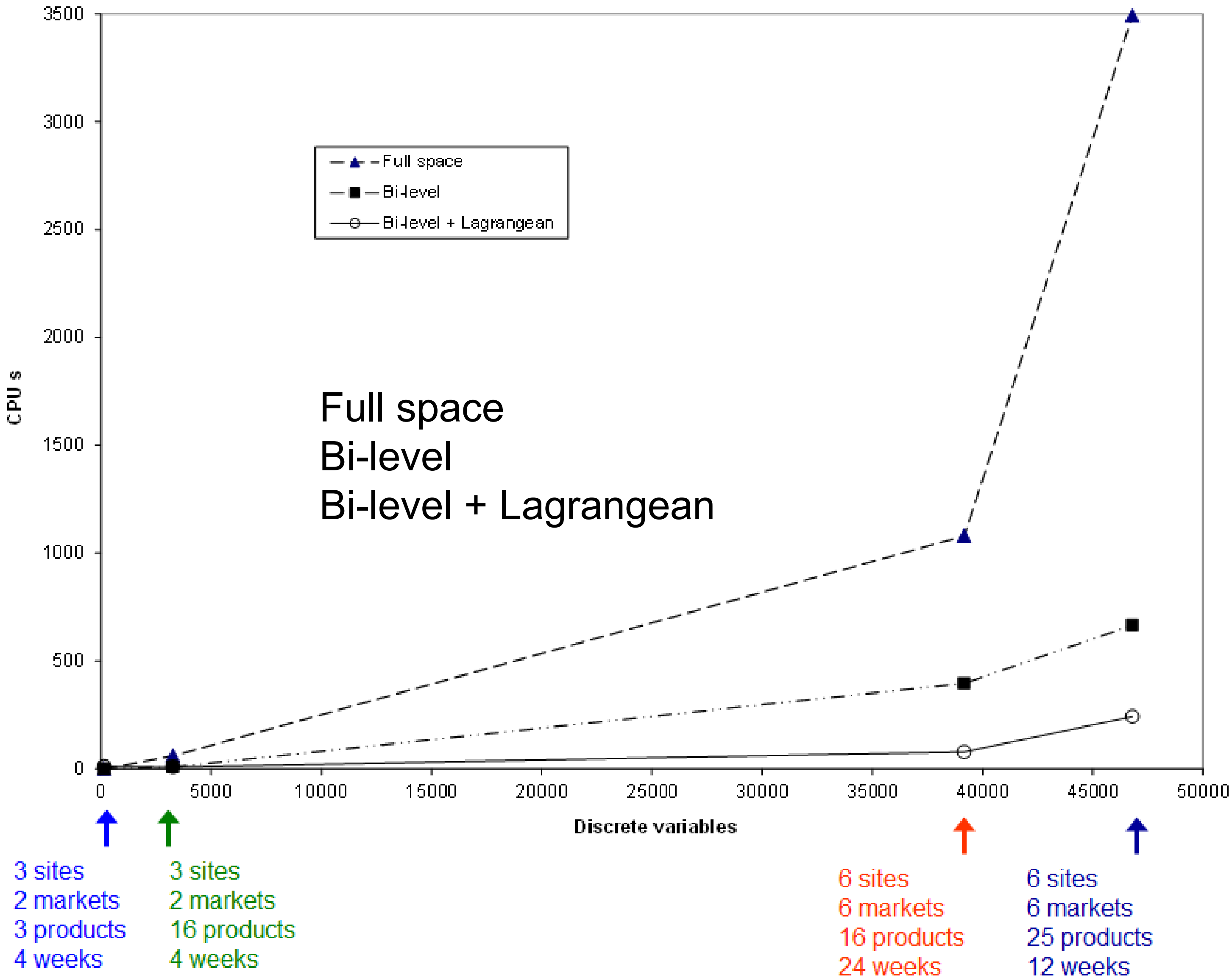
- **Bilevel decomposition**
  - Decouples planning from scheduling
  - Integrates across temporal scale
- **Lagrangean decomposition**
  - Decouples the solution of each production site
  - Integrates across spatial scale

Example: 3 sites, 3 products, 3 months

Profit: $ 2.576 million



Large-scale problems

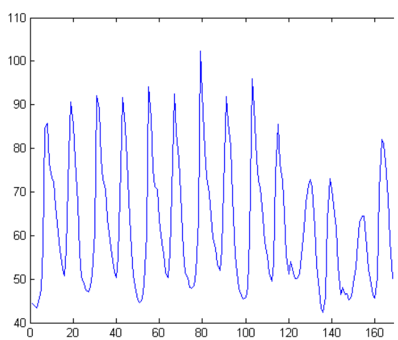


Electric Power Optimization in Air Separation Plant

Mitra, Grossmann, Pinto, Arora (2011)

Due to compressors!

Electricity Costs



Air Separation Plant

- **Liquid Oxygen**
- **Liquid Nitrogen**
- **Liquid Argon**
- **Gaseous Oxygen**
- **Gaseous Nitrogen**

Operational Decisions

- Which unit operate and amounts?
- Inventory levels?

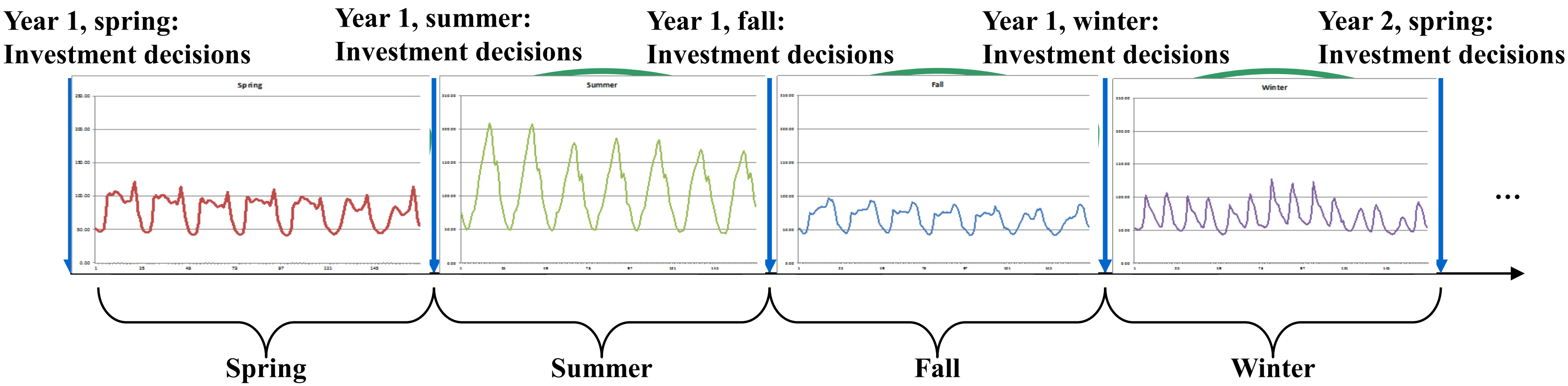
Strategic Decisions

- Additional liquefier?
- Additional tanks?
- Equipment upgrade?

Investment Costs

Multiscale design approach

Seasonal variations with cyclic weeks



- 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, configuration slates**
- Each representative week is repeated in a **cyclic** manner
  (For each season: **13** weeks reduced to **1** week) => **672** hrs vs **8736** hrs
- Connection between periods: Only through investment (design) decisions
- Design decisions are modeled by **discrete equipment sizes** => ***MILP***

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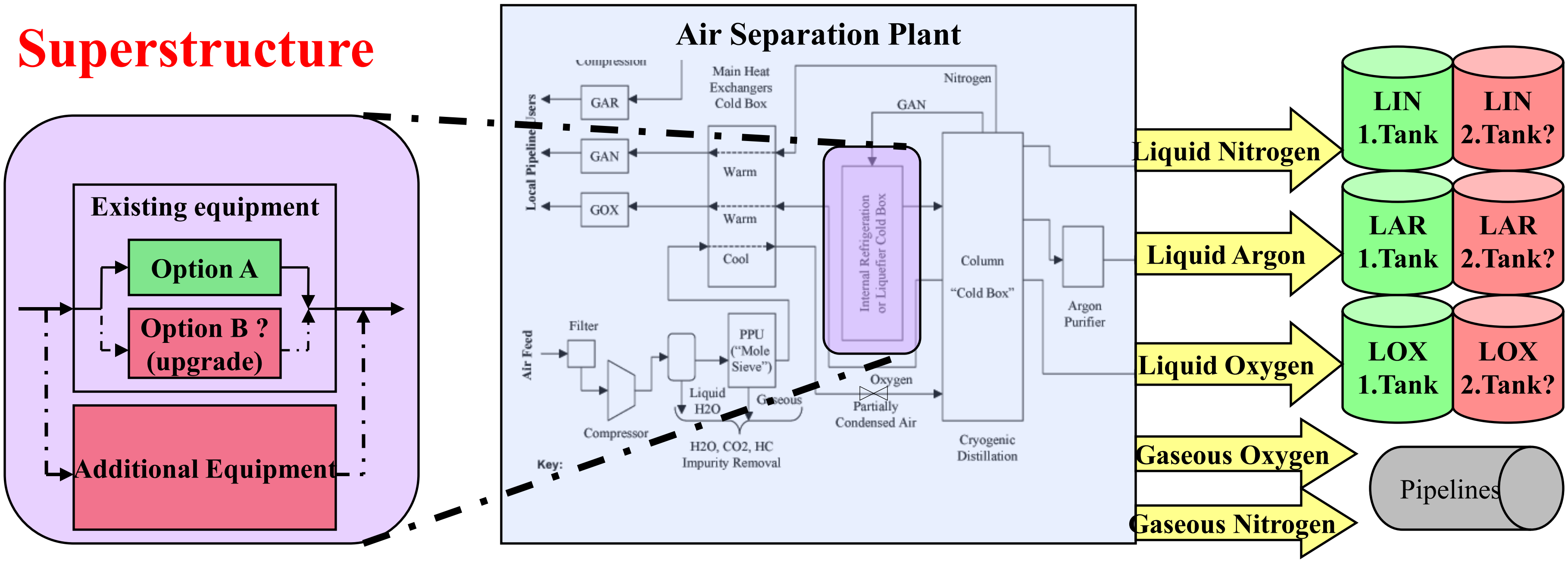
Retrofit air separation plant: selection and timing of design alternatives are degrees of freedom

Superstructure



Over one year with 4 periods

Optimal solution for added flexibility:

- **Buy the new equipment** in the first time period
- Do not upgrade the existing equipment
- Do not buy further storage tanks

Bi-level decomposition vs. full-space MILP problem

Computational times

Case	# Time periods (invest.)	Comments	# Constraints	# Variables	# Binary variables	Gap (difference between lower and upper bound)	CPU time (sec)
Full-space	4 **(1,3)**		**245,728**	**161,299**	**18,832**	**0.42%** (interrupted)	18,000 (interrupted)
Bi-level	4 **(1,3)**	**1 major iteration**: Only AP is solved a 2nd time (w cuts) to prove LB				**0%** **Between AP+DP**	**3814**
AP	4 **(1,3)**	1st iter, no cuts	**124,768**	**137,107**	**8,752**	0.08%	**841**
DP	4		**61,351**	**40,330**	**4,704**	0.07%	**503**

- Allowed integrality gap is 0.1%
- MIP Solvers: CPLEX 11.2.1, XPRESS (version: Aug 13 2009 for GAMS)
- Machine: Intel Centrino Duo, 2 Ghz

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- **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

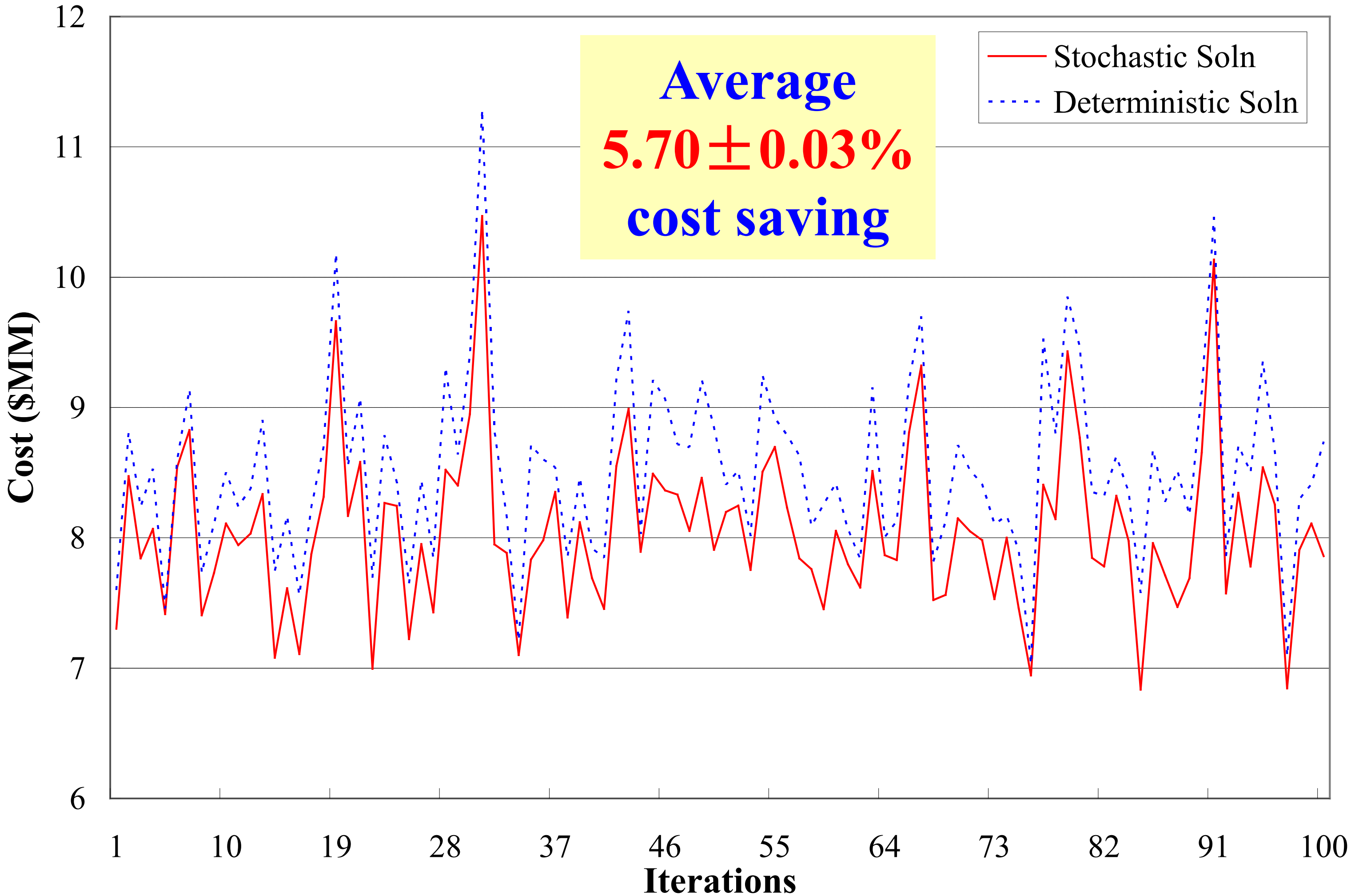
Case Study 1	Deterministic Model	Stochastic Programming Model
		1,000 scenarios
# of Constraints	62,187	52,684,187
# of Cont. Var.	89,014	75,356,014
# of Disc. Var.	7	7

- **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



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Optimal Development Planning under Uncertainty

Tarhan, Grossmann (2009)

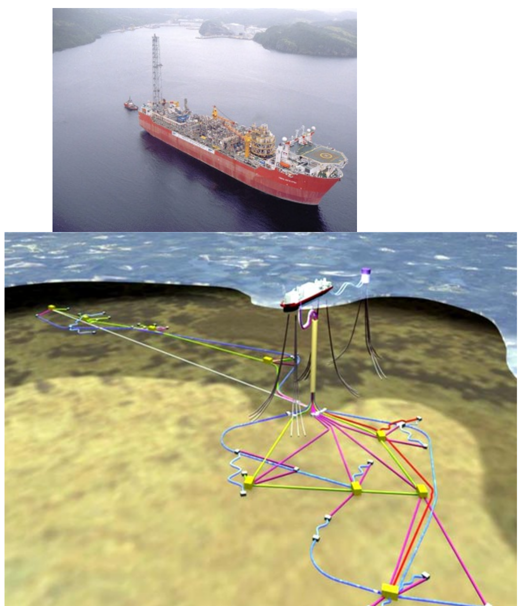
- **Offshore oilfield having several reservoirs under uncertainty**
- **Maximize the expected net present value (ENPV) of the project**

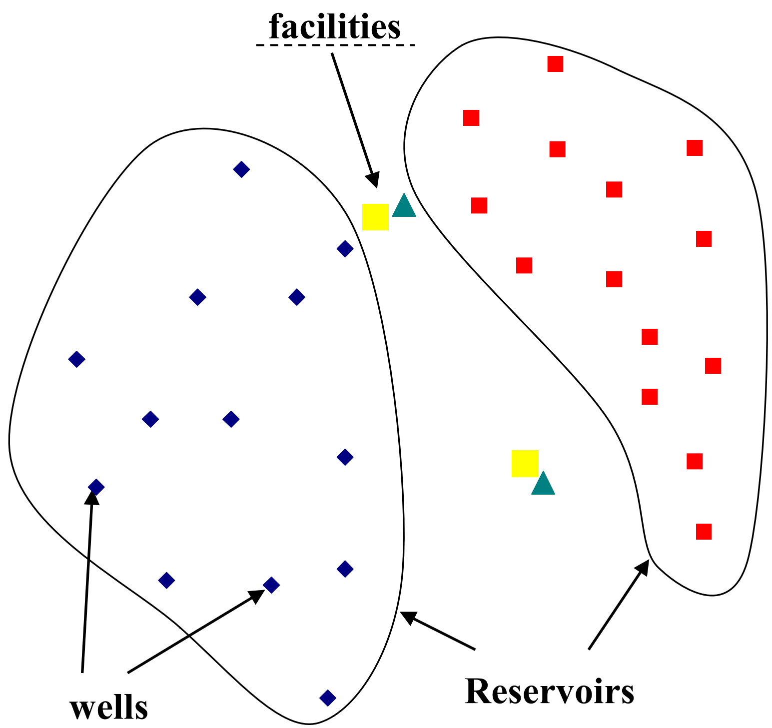
Decisions:

- 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





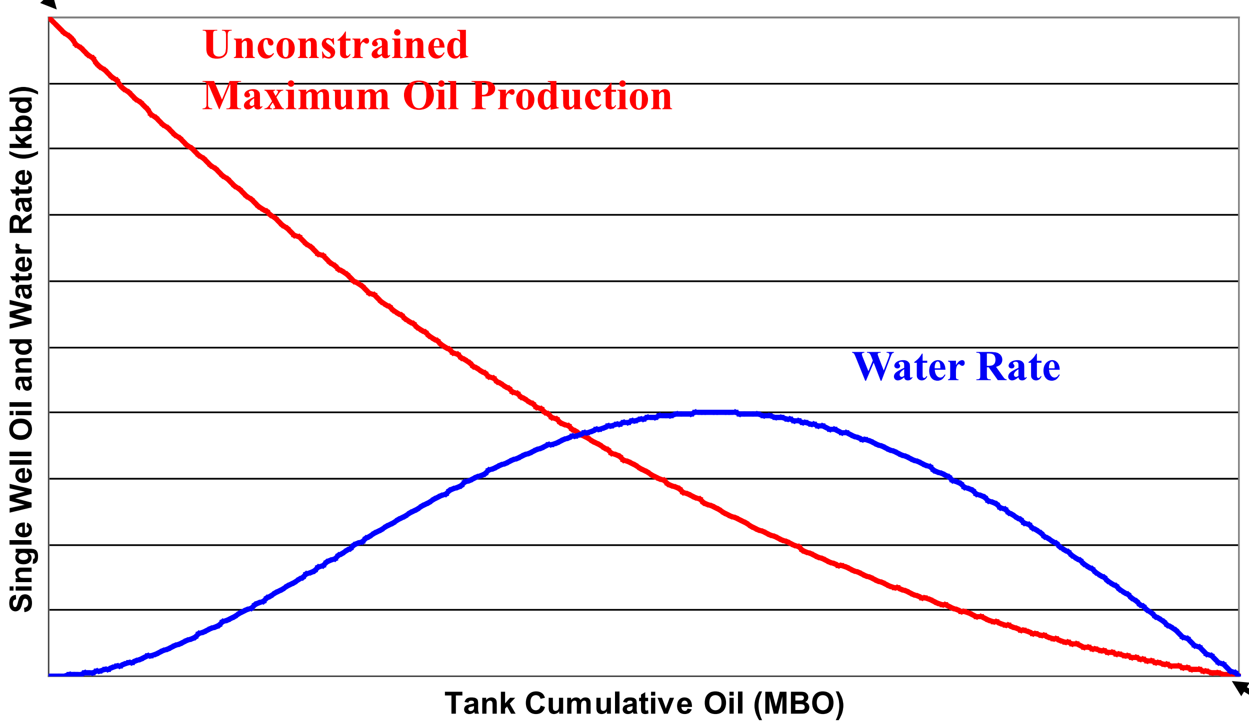
Uncertainty:

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

Non-linear Reservoir Model

Initial oil production

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



Size of the reservoir

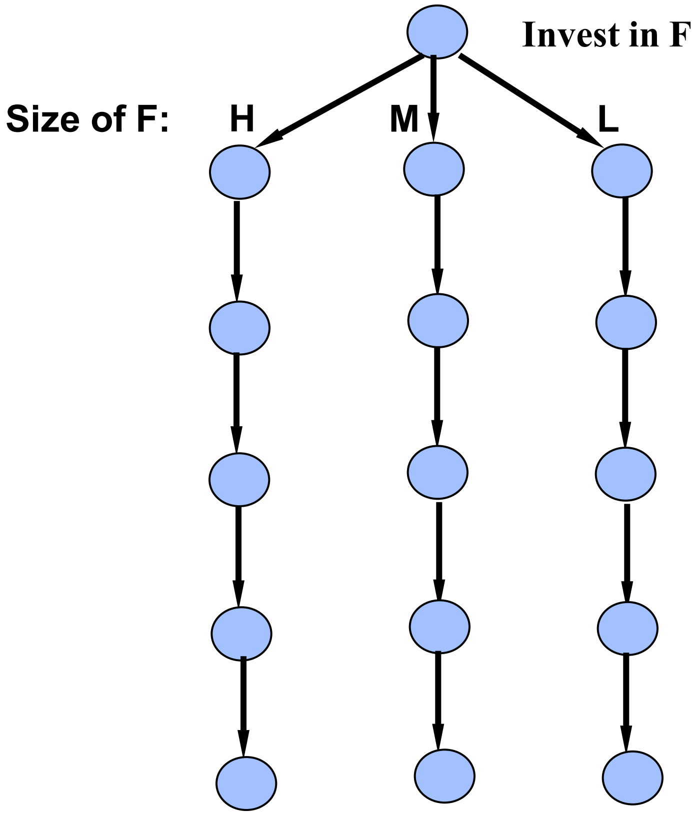
Uncertainty is represented by discrete distributions functions

Decision Dependent Scenario Trees

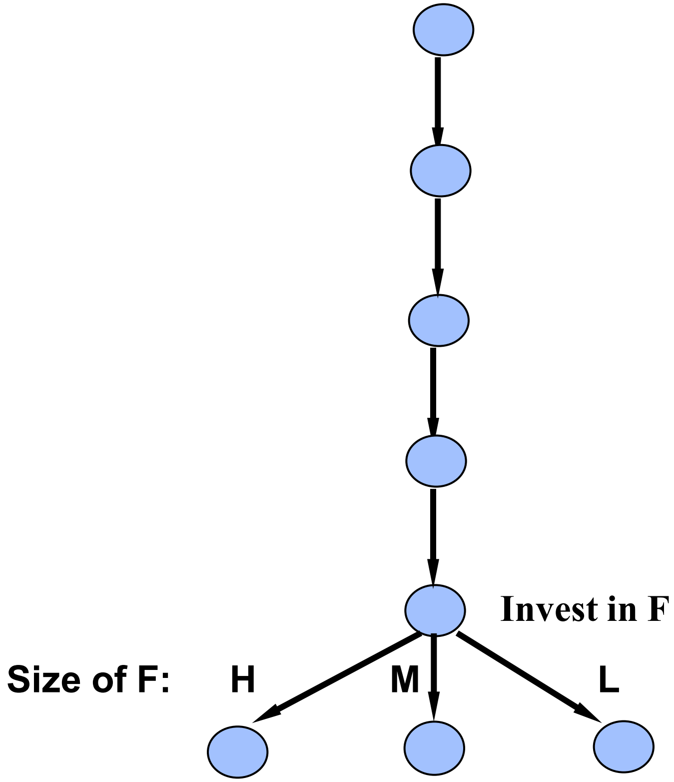
Endogeneous uncertainty: size field

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

Invest in F in year 1



Invest in F in year 5



Scenario tree

- **Not unique: Depends on timing of investment at uncertain fields**
- **Central to defining a Stochastic Programming Model**

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**

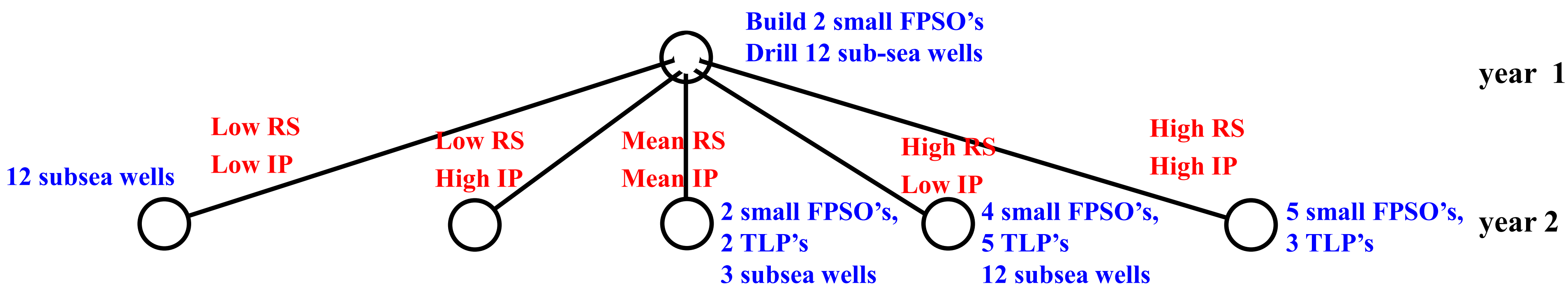
Problem size MINLP increases exponentially with number of time periods and scenarios	⇒	**Decomposition algorithm:** ***Lagrangean relaxation & Branch and Bound***

Multistage Stochastic Programming Approach

One reservoir, 10 years, 8 scenarios

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.

Multistage Stochastic Programming Approach

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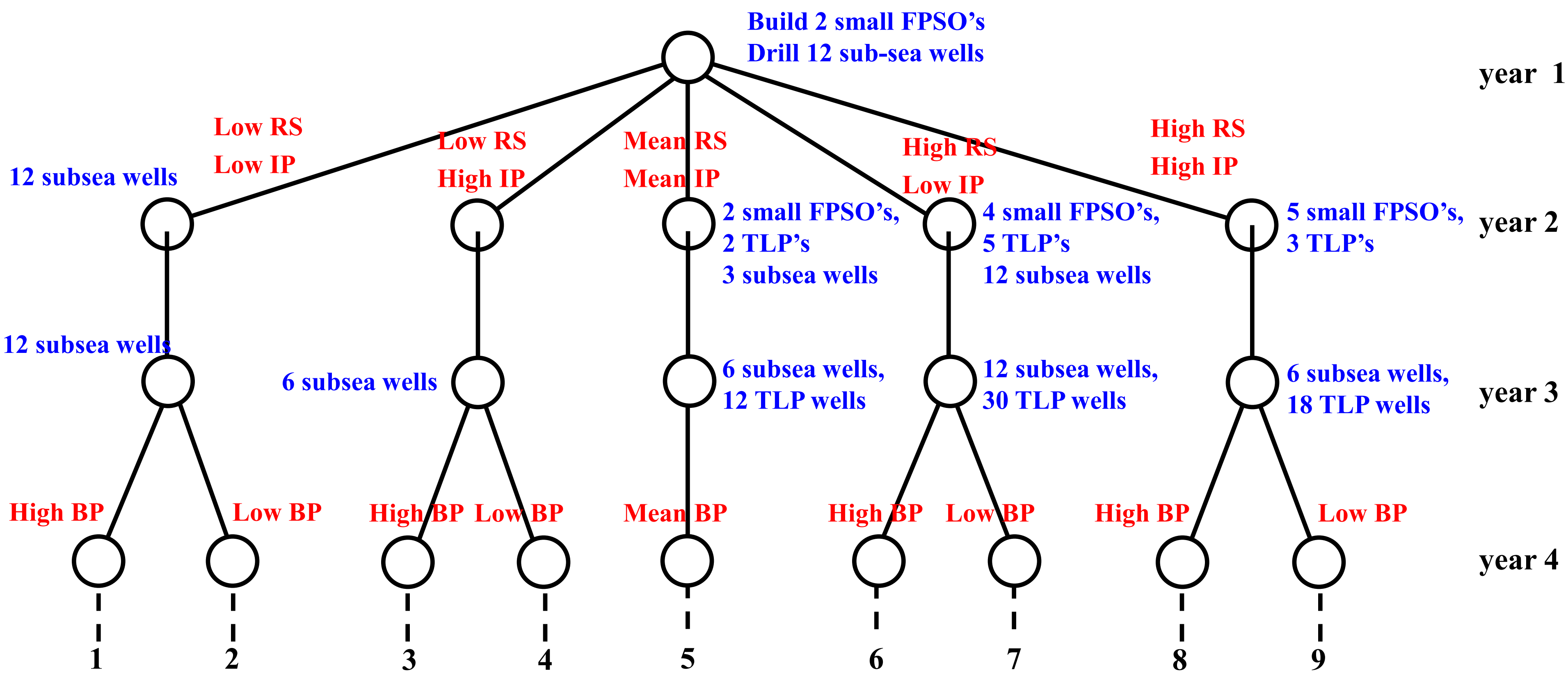

Solution proposes building **2** small FPSO's in the first year and then add new facilities / drill wells (**recourse action**) depending on the positive or negative outcomes.

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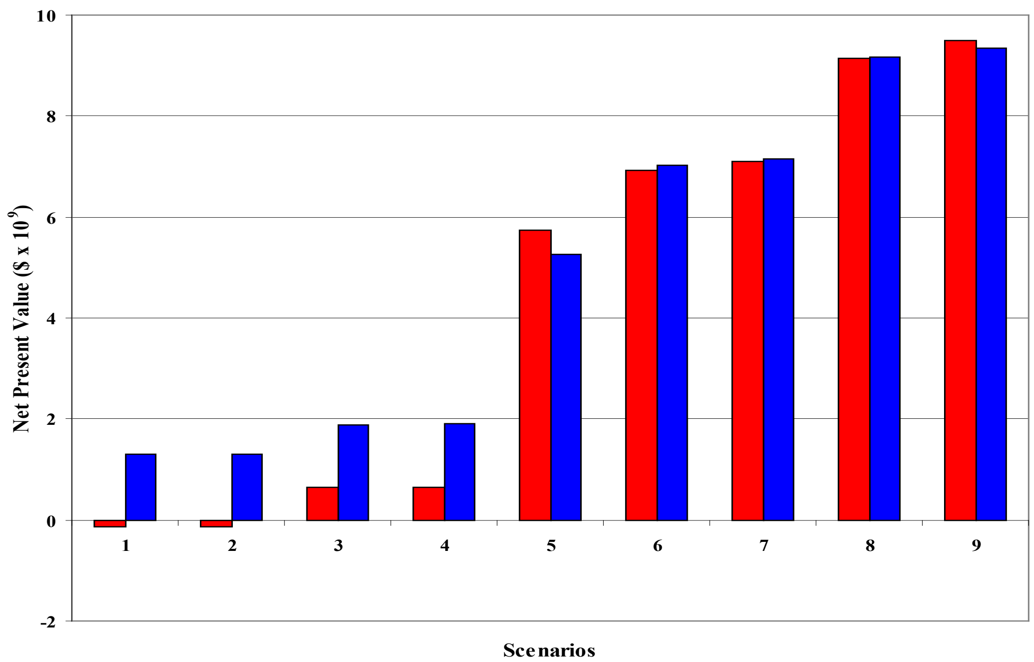
Distribution of Net Present Value



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

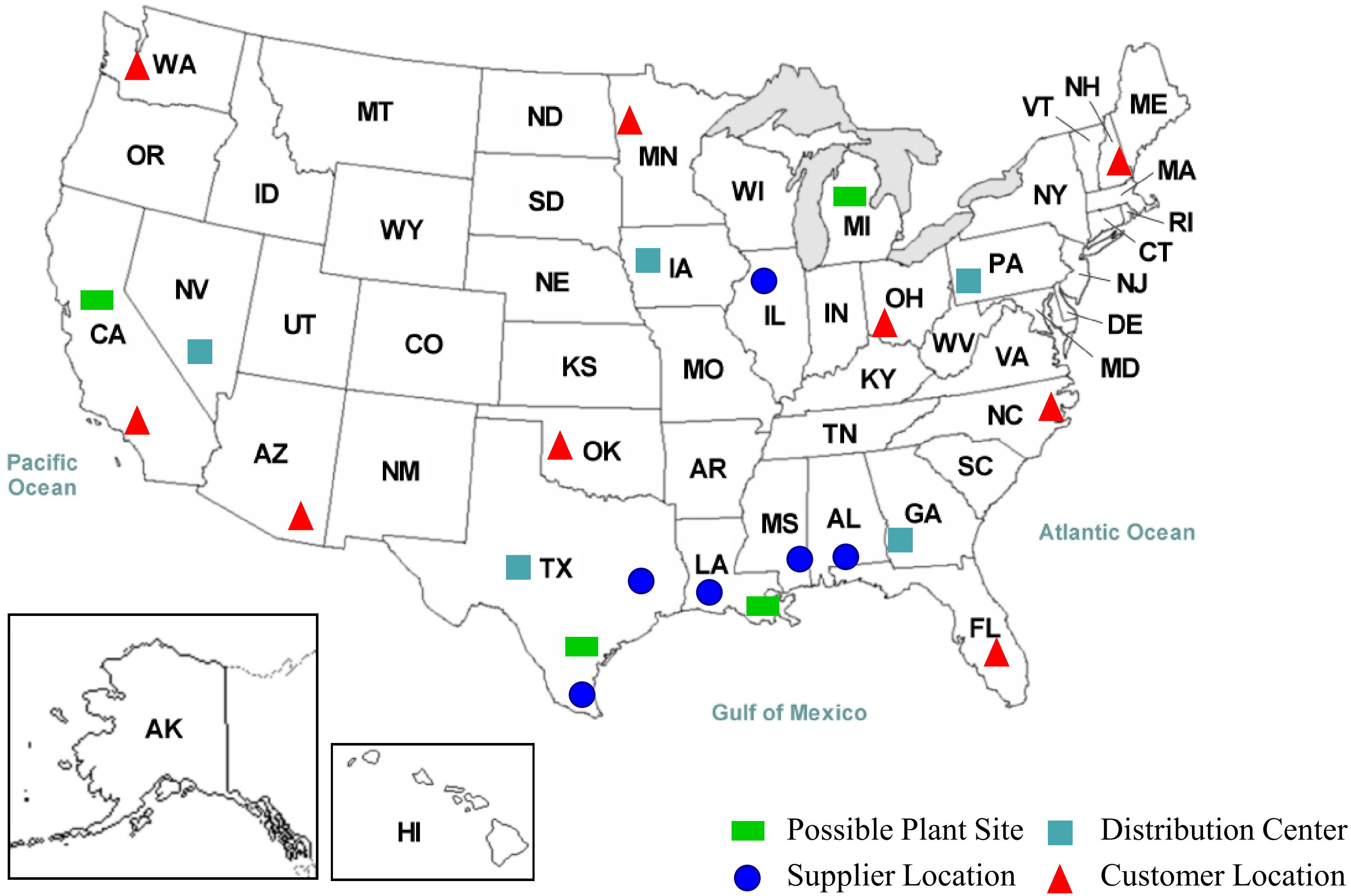
Economics vs. performance?

Multiobjective Optimization Approach

Optimal Design of Responsive Process Supply Chains

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

You, Grossmann (2008)



Production Network of Polystyrene Resins

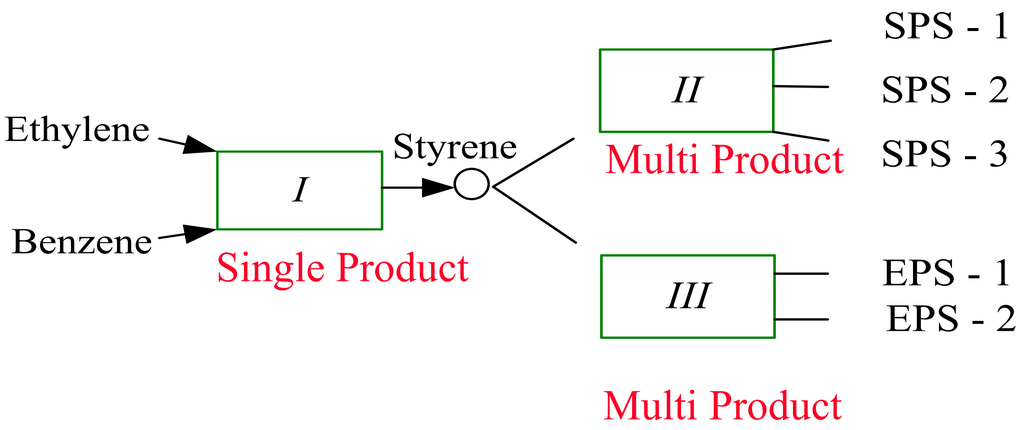
Three types of plants:

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



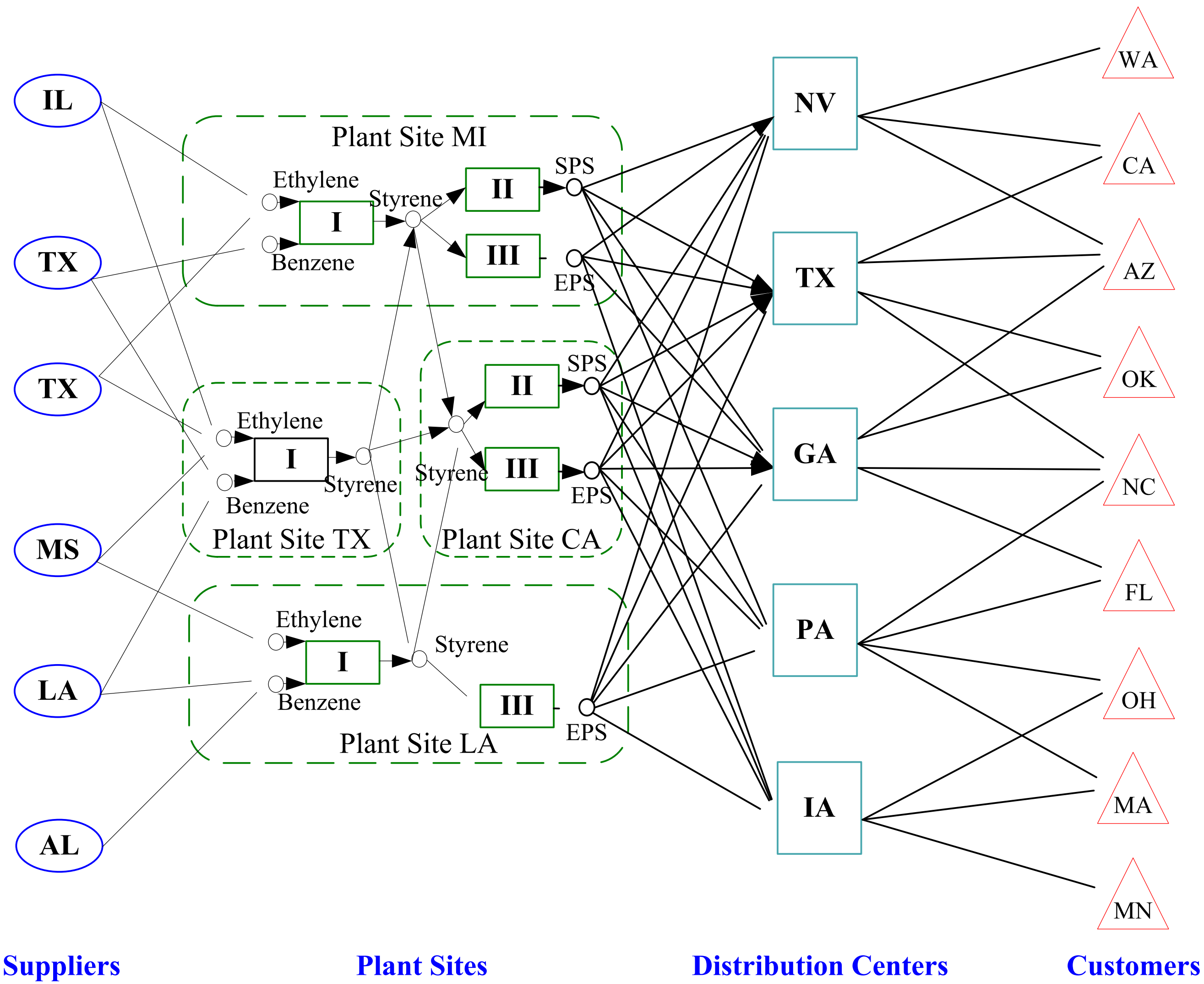
Source: Data Courtesy Nova Chemical Inc. http://www.novachem.com/

Example

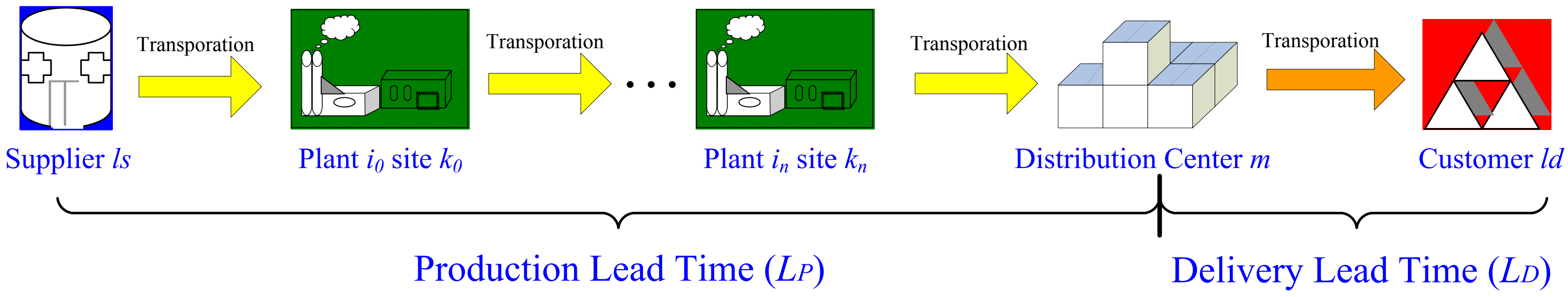
Chemical ENGINEERING

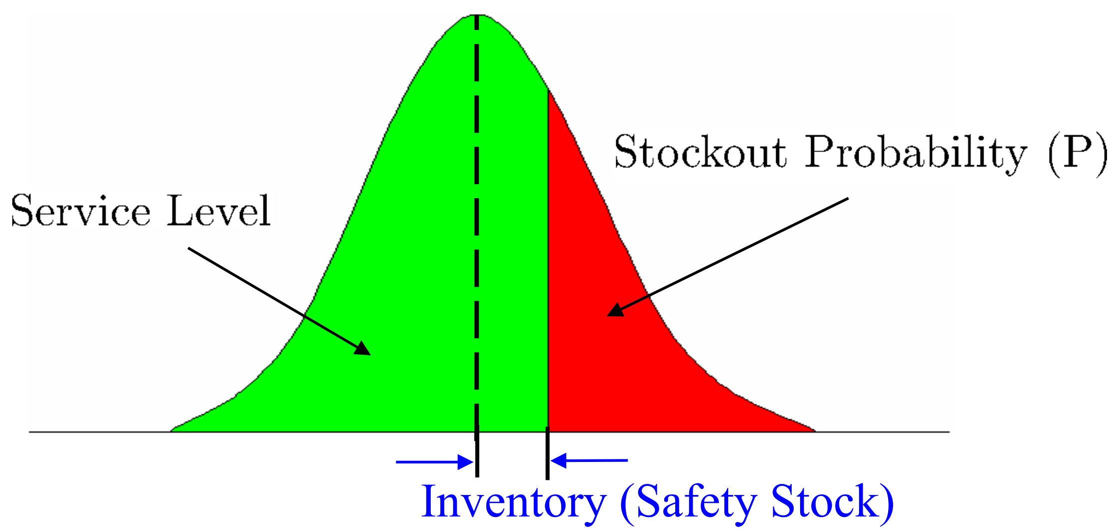
Potential Network Superstructure

CAPD CENTER



Lead Time under Demand Uncertainty





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

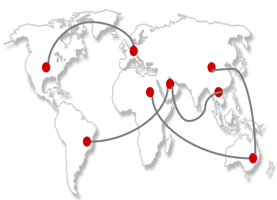
Bi-criterion Multiperiod MINLP Formulation

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

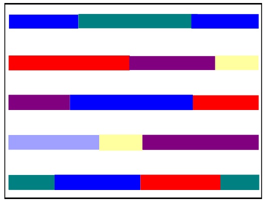
Capacity constraint

Mass balance constraint

Demand constraint

Upper bound constraint

  - Cyclic scheduling constraints



Assignment constraint

Sequence constraint

Demand constraint

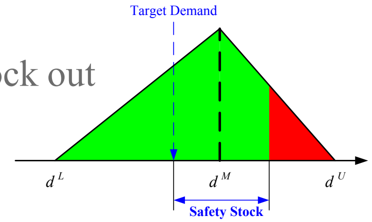
Production constraint

Cost constraint

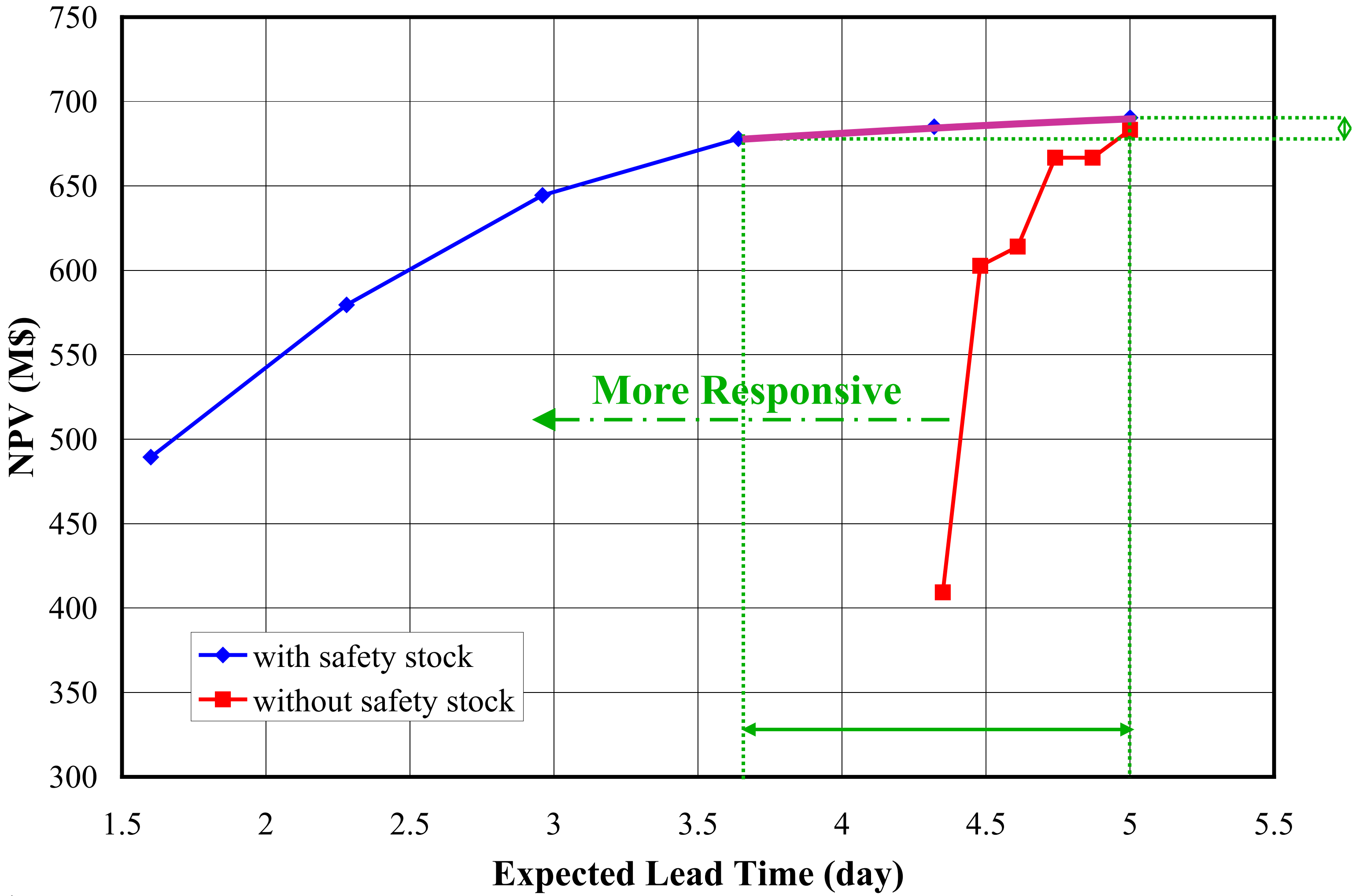
  - Probabilistic constraints

Chance constraint for stock out

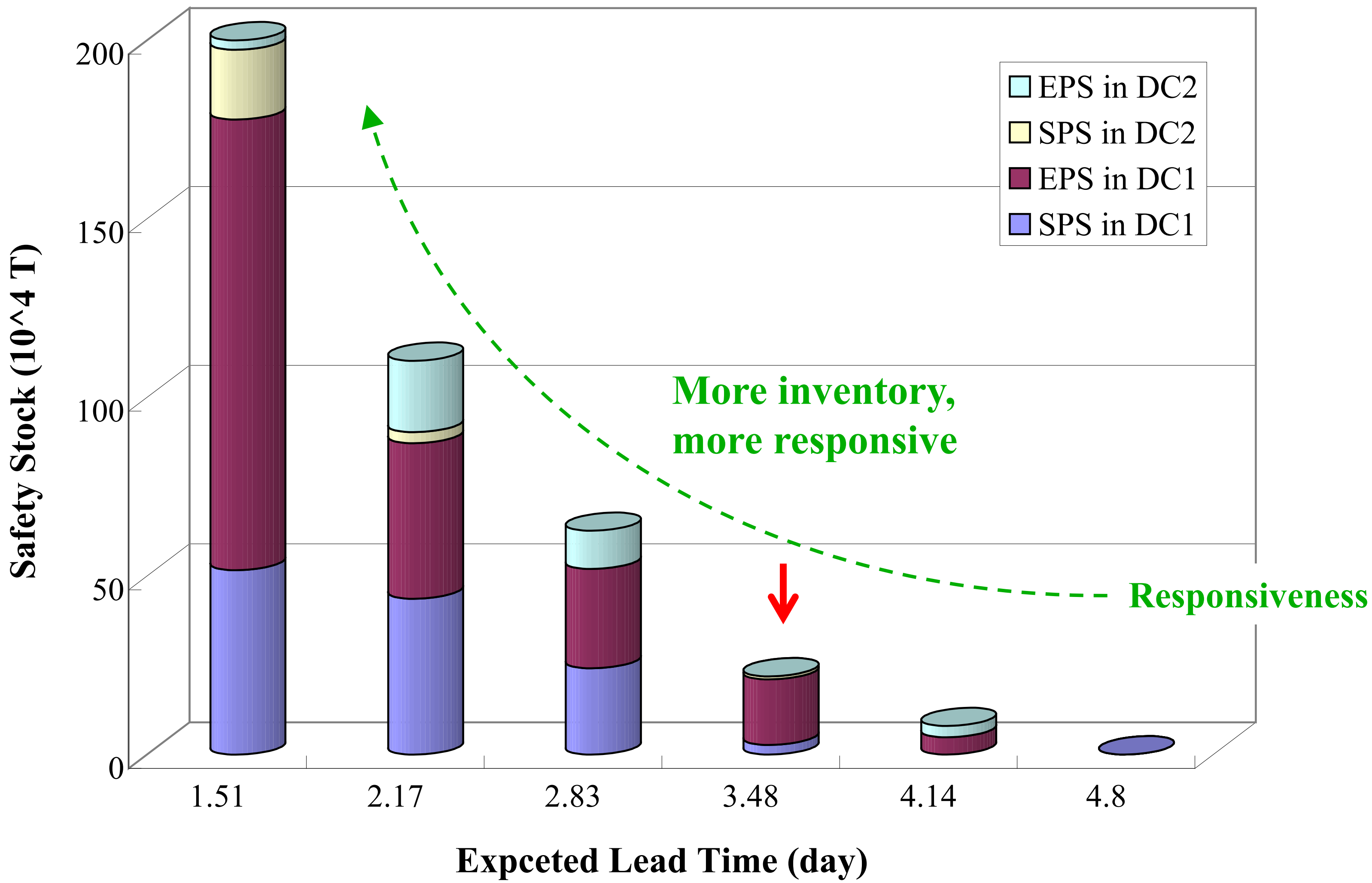
(reformulations)



Pareto Curves – with and without safety stock



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-Póvo, 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)