Mathematical Programming Approaches to Enterprise-wide Optimization of Process Industries

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Enterprise-wide Optimization (EWO)

EWO involves optimizing the operations of R&D, material supply, manufacturing, distribution of a company to <u>reduce costs and inventories</u>, and to <u>maximize profits, asset utilization, responsiveness</u> .

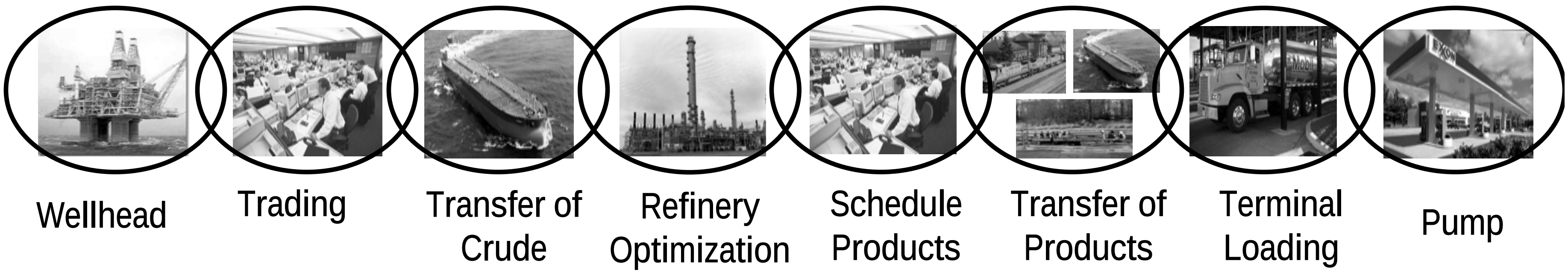
Grossmann, I. E., Enterprise-wide Optimization: A New Frontier in Process Systems Engineering. *AIChE Journal* 2005, 51, 1846-1857.

Varma, V. A.; Reklaitis, G. V.; Blau, G. E.; Pekny, J. F., Enterprise-wide modeling & optimization – An overview of emerging research challenges and opportunities. *Computers & Chemical Engineering* 2007, 31, 692-711.

Special Issue on Enterprise-wide Optimization,
(Eds. Ignacio Grossmann, Kevin Furman)
***Computers & Chemical Engineering* 2008 32, 2479-2838**

Petroleum industry

Dennis Houston (2003)



- **The supply chain is large, complex, and highly dynamic**
- **Optimization can have very large financial payout**

Pharmaceutical supply chain

R&D Pharmaceutical industry *(Gardner et al , 2003)*

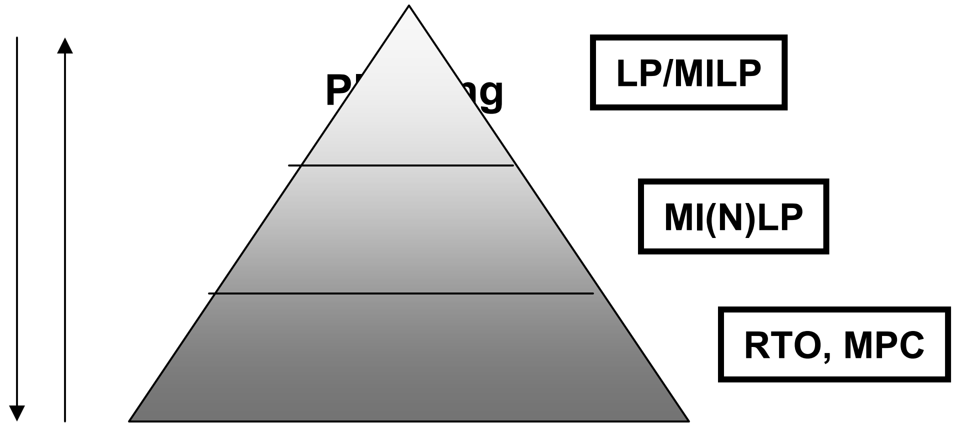
Discovery						Market
Targets Hits Leads Candidate	Pre-clinical Development	Phase 1	Phase 2a/b	Phase 3	Submission& Approval	Lifecycle Management
2-5 yrs	0.5 - 2 yrs	1 - 2 yrs	1.5 - 3.5 yrs	2.5 - 4 yrs	0.5-2 yrs	10-20 yrs

- **Pharmaceutical process** *(Shah, 2003)*
  - Primary production has five synthesis stages
  - Two secondary manufacturing
  - Global market

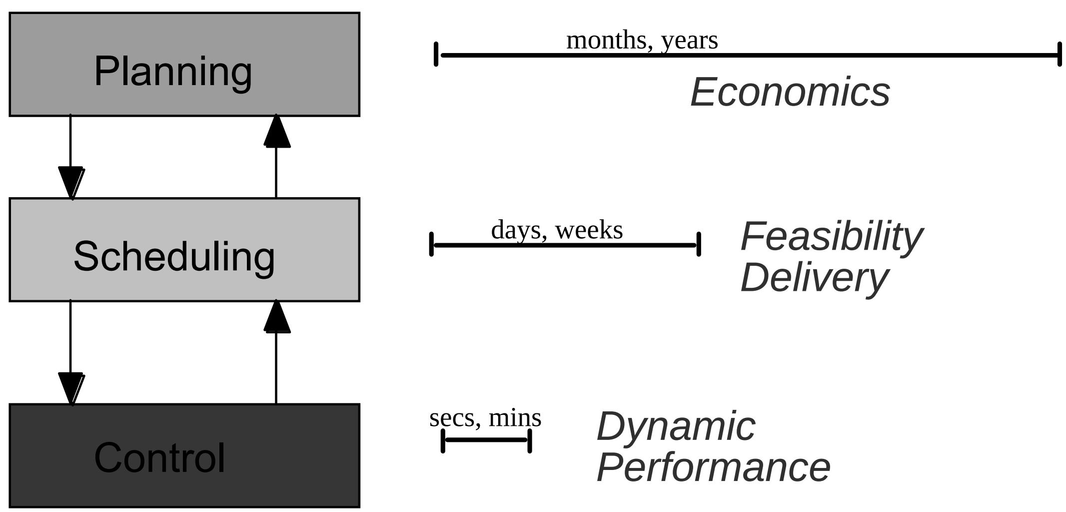
Key issues:

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

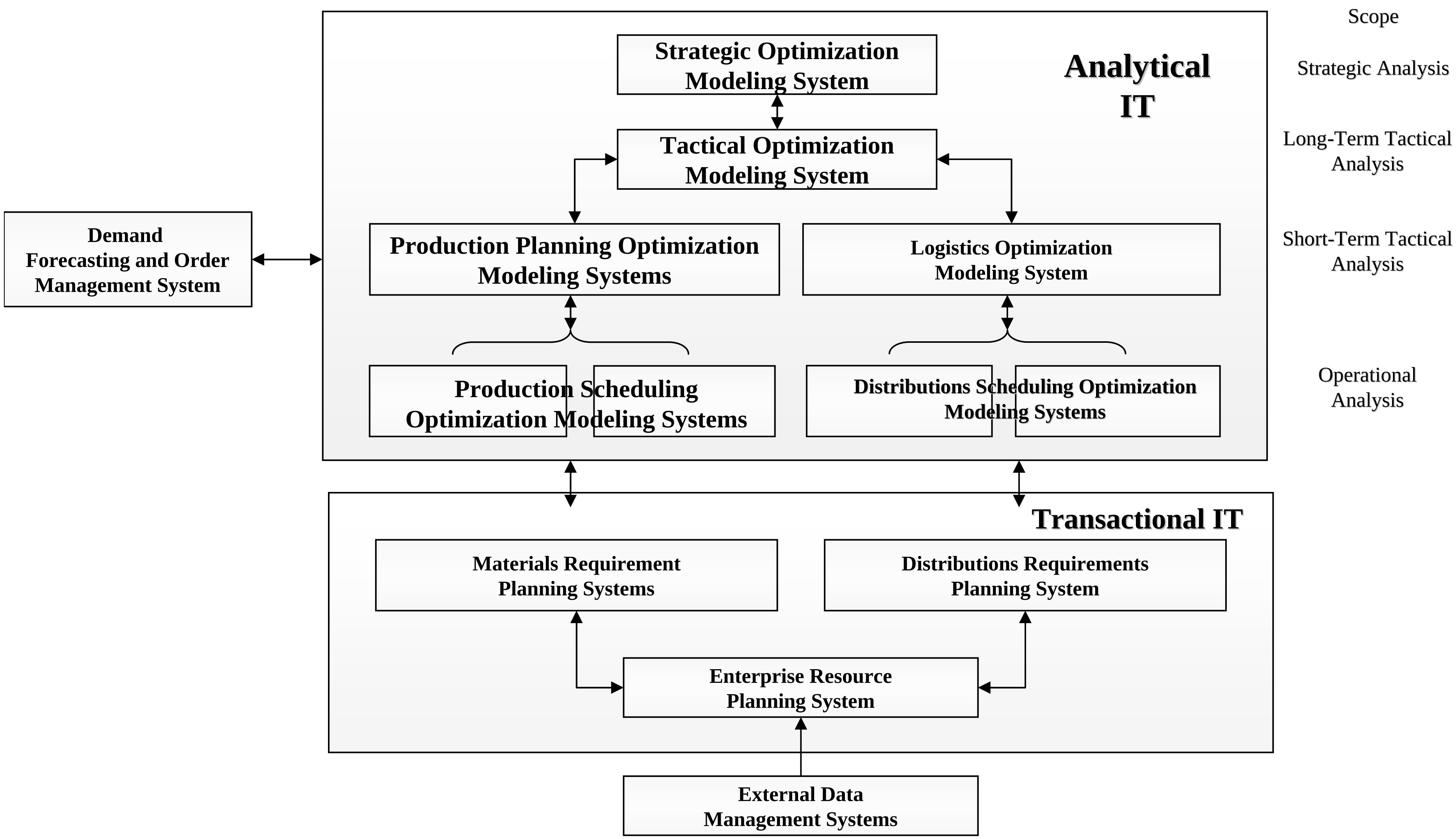
<u>Mutiple models</u>



<u>Mutiple time scales</u>



II. Integration of information, modeling and solution methods



Source: Tayur, et al. [1999]

Research Challenges

-The modeling challenge:

Planning, scheduling, control models **for the various components of the supply chain, including** ***nonlinear process*** **models?**

- The multi-scale optimization challenge:

Coordinated planning/scheduling models over ***geographically distributed*** **sites, and over the** ***long-term*** **(years),** ***medium-term*** **(months) and** ***short-term*** **(days, min) decisions?**

- The uncertainty challenge:

How to effectively anticipate effect of ***uncertainties*** **?**

- Algorithmic and computational challenges:

How to ***effectively solve large-scale*** **models including** ***nonconvex problems*** **in terms of efficient algorithms, and modern computer architectures?**

Enterprise-wide Optimization

Multidisciplinary team:

Chemical engineers, Operations Research, Industrial Engineering

Researchers:	
Carnegie Mellon:	**Ignacio Grossmann (ChE)**
	Larry Biegler (ChE)
	John Hooker (OR)
	Nicola Secomandi (OR)
Lehigh University:	**Larry Snyder (Ind. Eng)**
Univ. Pittsburgh:	**Andrew Schaeffer (Ind. Eng.)**

Examples of EWO problems

Simultaneous Tactical Planning and Production Scheduling

Dow Chemical

Large-scale mixed integer linear programming

Supply Chain Design with Stochastic Inventory Management

Nonconvex mixed-integer nonlinear program

Optimization Under Uncertainty for Off-shore Oilfield Planning

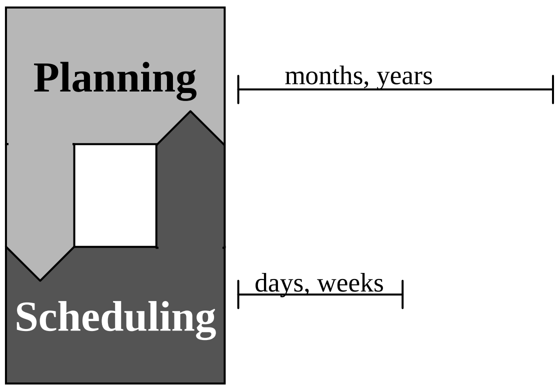
ExxonMobil

Stochastic Programming with variable scenario trees

Integration of Planning and Scheduling

Decomposition

Sequential Hierarchical Approach

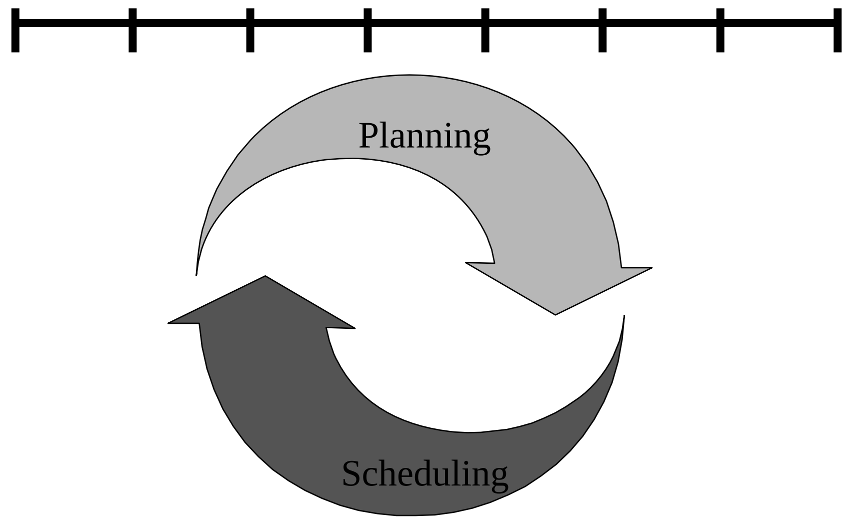


Challenges:

- ✓ Different models / different time scales
- ✓ **Mismatches between the levels**

Simultaneous Planning and Scheduling

Detailed scheduling over the entire horizon



Challenges:

- ✓ Very Large Scale Problem
- ✓ **Solution times quickly intractable**

Goal: Aggregate Planning model that integrates major aspects of scheduling

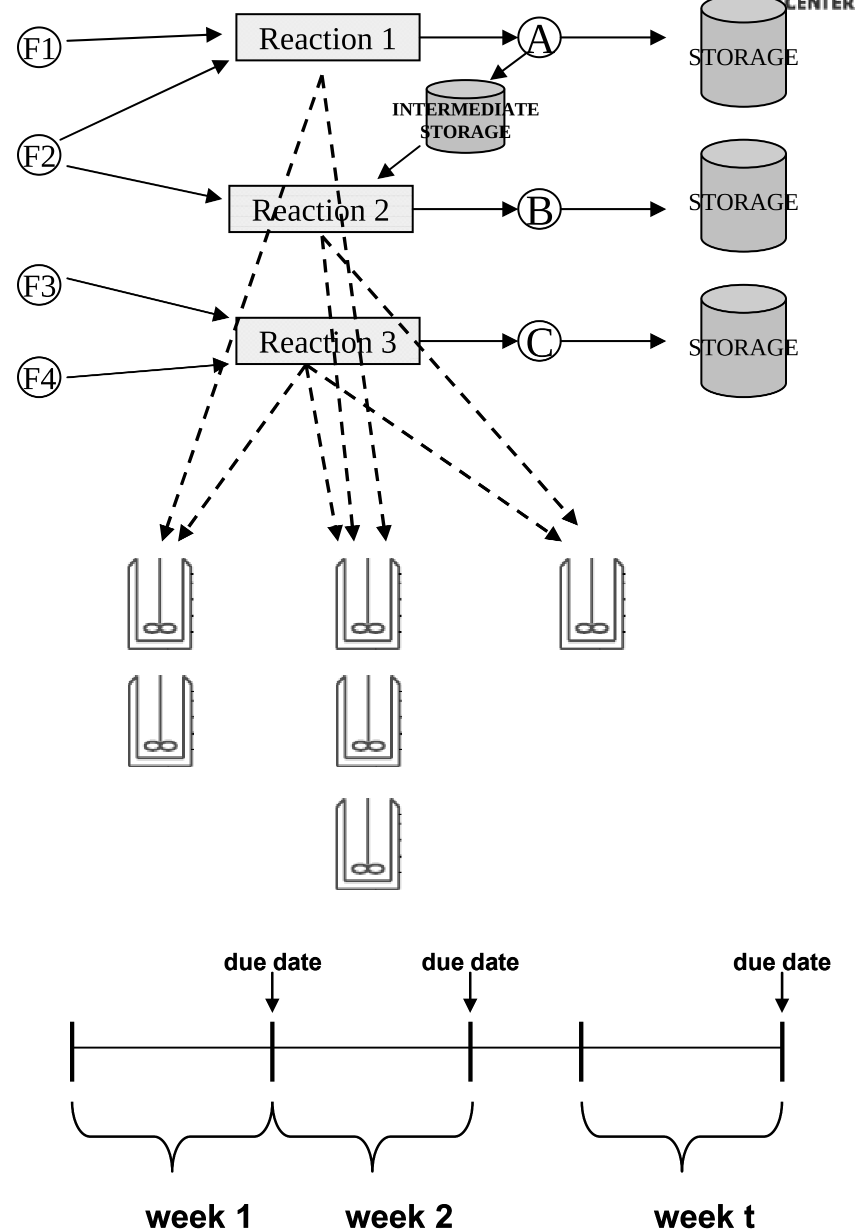
Production Planning for Parallel Batch Reactors

Erdirik, Grossmann & Wassick(2007)

Materials:
- Raw materials, Intermediates, Finished products
- Unit ratios (lbs of needed material per lb of material produced)

Production Site:
- Reactors:
  - Products it can produce
  - **Batch sizes** for each product
  - **Batch process time** for each product (hr)
  - Operating costs ($/hr) for each material
  - ***Sequence dependent change-over times /costs***
  - ***=> Lost capacity***
    (hrs per transition for each material pair)
  - Time the reactor is available during a given month (hrs)

Customers:
- Monthly forecasted demands for desired products
- Price paid for each product



Problem Statement

DETERMINE THE PRODUCTION PLAN:

- ✓ Production quantities
- ✓ Inventory levels
- ✓ Number of batches of each product
- ✓ Assignments of products to available processing equipment
- ✓ ***Sequence of production*** in each processing equipment

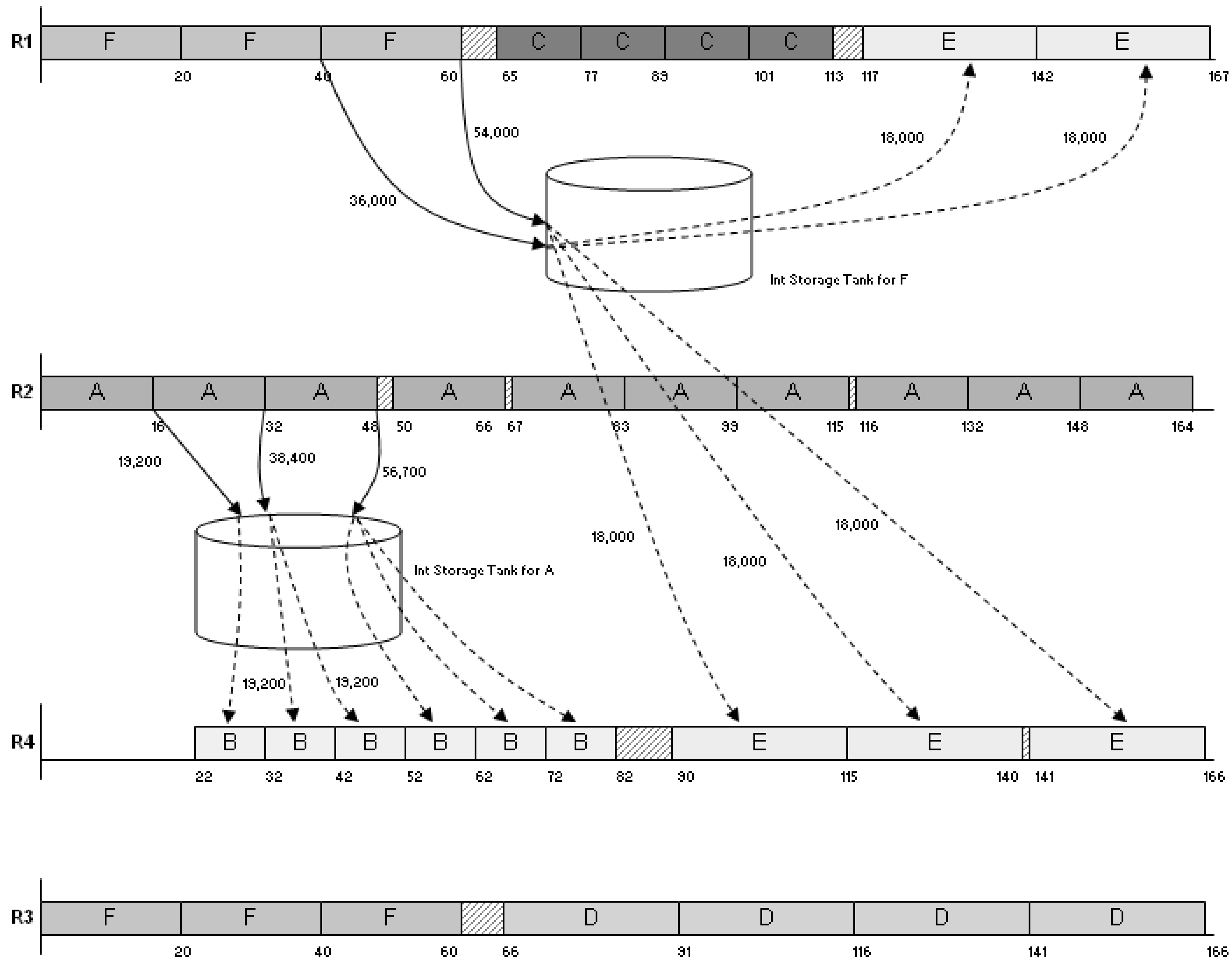
OBJECTIVE:

To Maximize **Profit**.

Profit = Sales – Costs

Costs=Operating Costs + Inventory Costs +Transition Costs

Results for Detailed MILP Scheduling Model: 4 reactors,6 products (1 week)



MILP Detailed Scheduling Model

Objective Function:

$$Profit = \sum_i \sum_t CP_{i,t} \cdot S_{i,t} - \sum_i \sum_m \sum_l \sum_t COP_{i,t} \cdot XB_{i,m,l,t} - \sum_i \sum_t CINV_{i,t} \cdot (INV_{i,t} + INVFIN_{i,t} + INVINT_{i,t}) - \sum_i \sum_k \sum_m \sum_l \sum_t CTRA_{i,k} \cdot \left(Z_{i,k,m,l,t} + \tilde{Z}_{i,k,m,l,t} + \hat{Z}_{i,k,m,l,t} \right)$$

Assignment constraints and Processing times:

$$\sum_i W_{i,m,l,t} \le 1 \quad i \in IM(m), \forall\, l \in (L(m) \cap L(t)), \forall m, \forall t$$

$$\sum_{i \in IM(m)} W_{i,m,l,t} \ge \sum_{i \in IM(m)} W_{i,m,l,t} \quad \forall l \in (L(m) \cap L(t)), l \ne N(t), \forall m, \forall t$$

$$PT_{i,m,l,t} = BT_{i,m} \cdot W_{i,m,l,t} \quad \forall i \in IM(m), \forall l \in (L(m) \cap L(t)), \forall m, \forall t$$

$$X_{i,m,l,t} = R_{i,m} \cdot BT_{i,m} \cdot W_{i,m,l,t} \quad \forall i \in IM(m), \forall l \in (L(m) \cap L(t)), \forall m, \forall t$$

Detailed timing constraints and sequence dependent change :

$$Z_{i,i',m,l,t} \ge W_{i,m,l,t} + W_{i',m,l+1,t} - 1 \quad \forall i \in IM(m), \forall i' \in IM(m), i' \ne i, \forall l \in (L(m) \cap L(t)), l \ne Nt, \forall m, \forall t$$

$$TR_{m,l,t} = \sum_i \sum_{i'} \tau_{i,i'} \cdot Z_{i,i',m,l,t} \quad \forall l \in (L(m) \cap L(t)), l \ne Nt, \forall m, \forall t$$

$$\tilde{Z}_{i,i',m,l,t} \ge W_{i,m,l,t} + W_{i',m,'1',t+1} - 1 \quad \forall i, i' \in IM(m), i' \ne i, \forall l \in (L(m) \cap L(t)), \forall m, \forall t, t \ne H_t$$

$$Te_{m,l,t} = Ts_{m,l,t} + \sum_i PT_{i,m,l,t} + \sum_i \sum_k \tau_{i,k} \cdot Z_{i,k,m,l,t} + TRT_{m,l,t} - TX_{m,l,t} + \left(\sum_i \sum_{i'} \tau_{i,i'} \cdot \hat{Z}_{i,i',m,l,t}\right) \quad \forall m, l, t$$

$$TRT_{m,l,t} = TRT1_{m,l,t} + TRT2_{m,l,t} \quad \forall m, l, t$$

$$TX_{m,l,t} = TRT1_{m,l,t} \quad \forall m, l, t$$

$$TRT1_{m,l,t} \le UPPER \cdot Y_{m,l+1,t} \quad \forall m, l, t$$

$$TRT2_{m,l,t} \le UPPER \cdot (1 - Y_{m,l+1,t}) \quad \forall m, l, t$$

MILP Detailed Scheduling Model

Mass and Inventory Balances:

$$X_{i,m,l,t} = INVP^{FIN}_{i,m,l,t} + INVINT^{TRA}_{i,m,l,t} \qquad i \in IFINT_i, \forall l \in (L(m) \cap L(t)), \forall m, \forall t$$

$$INVINT^{TRA}_{i,m,l,t} = INVP^{INT}_{i,m,l,t} + \sum_{l'>l, l' \in L(m)} AA_{i,m,l,m,l',t} + \sum_{m' \neq m} \sum_{l' \in L(m')} AA_{i,m,l,m',l',t} \qquad i \in IFINT_i, \forall l \in (L(m) \cap L(t)), \forall l' \in L(t), \forall m, \forall m' \neq m, \forall t$$

$$X_{i,m,l,t} = INVP^{FIN}_{i,m,l,t} + INVP^{INT}_{i,m,l,t} + \sum_{l'>l, l' \in L(m)} AA_{i,m,l,m,l',t} + \sum_{m' \neq m} \sum_{l' \in L(m')} AA_{i,m,l,m',l',t} \qquad i \in IFINT_i, \forall l \in (L(m) \cap L(t)), \forall l' \in L(t), \forall m, \forall m' \neq m, \forall t$$

$$Ts_{m,l,t} + \sum_{i} PT_{i,m,l,t} \le Ts_{m',l',t} + BigW_t \cdot (1 - YY_{l,l',m,m',t}) \qquad \forall l \in (L(m) \cap L(t)), \forall l' \in (L(m') \cap L(t)), \forall m, \forall m' \neq m, \forall t$$

$$Ts_{m',l',t} \le Ts_{m,l,t} + \sum_{i} PT_{i,m,l,t} + BigW_t \cdot (YY_{l,l',m,m',t}) \qquad \forall l \in (L(m) \cap L(t)), \forall l' \in (L(m') \cap L(t)), \forall m, \forall m' \neq m, \forall t$$

$$AA_{i,m,l,m',l',t} \le UBOUND_i \cdot (YY_{l,l',m,m',t}) \qquad i \in IFINT_i, \forall l \in (L(m) \cap L(t)), \forall l' \in (L(m') \cap L(t)), \forall m, \forall m' \neq m, \forall t$$

$$\sum_{m' \neq m} \sum_{l' \in (L(m') \cap L(t))} AA_{i,m,l,m',l',t} \le UBOUND_i \cdot (W_{i,m,l,t}) \qquad i \in IFINT_i, \forall l \in (L(m) \cap L(t)), \forall m, \forall t$$

$$\sum_{l' \in (L(m) \cap L(t))} AA_{i,m,l,m',l',t} \le UBOUND_i \cdot (W_{i,m,l,t}) \qquad i \in IFINT_i, \forall l \in (L(m) \cap L(t)), \forall m, \forall t$$

$$AA_{i,m,l,m',l',t} \le UPBOUND_{i,m} \cdot \sum_{i' \in ENDINT(i',i)} (W_{i',m,l,m',l',t}) \qquad i \in IFINT_i, \forall l \in (L(m) \cap L(t)), \forall l' \in (L(m') \cap L(t)), \forall m, \forall m' \neq m, \forall t$$

$$INV^{INT}_{i,t-1} + \sum_{m} \sum_{l \in (L(m) \cap L(t))} INVP^{INT}_{i,m,l,t} = \sum_{m} \sum_{l \in (L(m) \cap L(t))} INVC_{i,m,l,t} + INV^{INT}_{i,t} \qquad i \in IFINT_i, \forall t$$

$$INV^{FIN}_{i,t-1} + \sum_{m} \sum_{l \in (L(m) \cap L(t))} INVP^{FIN}_{i,m,l,t} = S_{i,t} + INV^{FIN}_{i,t} \qquad i \in IFINT_i, \forall t$$

$$X_{i,m,l,t} = \sum_{i'} \alpha_{i,i'} \cdot \Big(INVC_{i',m,l,t} + \sum_{\substack{l''<l \\ l' \in (L(m) \cap L(t))}} AA_{i,m,l'',m,l,t} + \sum_{m' \neq m} \sum_{l' \in (L(m') \cap L(t))} AA_{i,m',l',m,l,t}\Big) \qquad i \in IE_i, \forall l \in (L(m) \cap L(t)), \forall m, \forall t$$

$$INV^{FIN}_{i,t-1} + \sum_{m} \sum_{l \in (L(m) \cap L(t))} X_{i,m,l,t} = S_{i,t} + INV^{FIN}_{i,t} \qquad i \in (IE_i \cup IF_i), \forall t$$

Proposed Aggregate MILP Planning Models

Replace the detailed timing constraints by:

Model A. (Relaxed Planning Model)

- ✓ Constraints that **underestimate the sequence dependent** changeover times
- ✓ **Weak** upper bounds **(Optimistic Profit)**

Model B. (Detailed Planning Model)

- ✓ **Sequencing constraints** for accounting for transitions rigorously
  (Traveling salesman constraints)
- ✓ **Tight** upper bounds **(Realistic estimate Profit)**

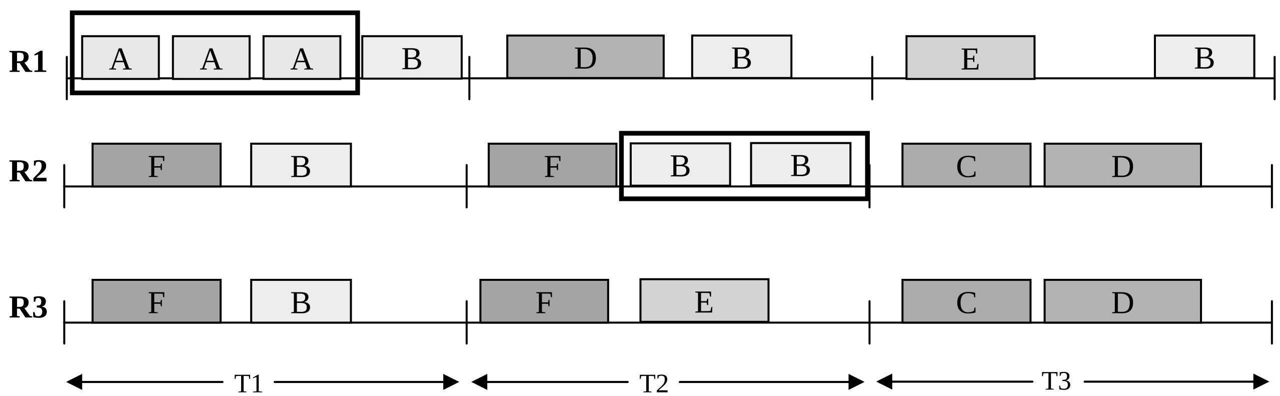
Key Variables for MILP Planning Model

$YP_{i,m,t}$:the assignment of products to units at each time period

NB_{imt} :number of each batches of each product on each unit at each period

FP_{imt} :amount of material processed by each task

Products: A, B, C, D, E, F → Reactor 1 or Reactor 2 or Reactor 3



$$YP_{A,reactor1,time1} = 1$$
$$NB_{A,reactor1,time1} = 3$$

$$YP_{B,reactor2,time2} = 1$$
$$NB_{B,reactor2,time2} = 2$$

Proposed Model B (Detailed Planning)

Sequence dependent changeovers (traveling salesman constraints):

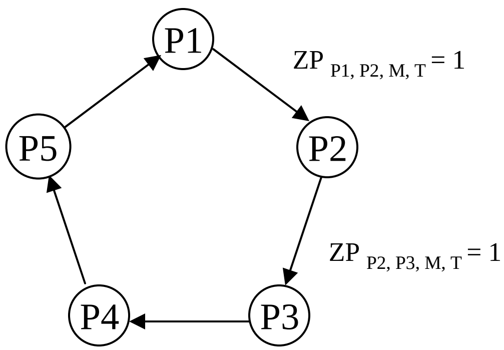
✓ **Changeovers within each time period:**

1. **Generate a cyclic schedule where total transition time is minimized.**

KEY VARIABLE:

$ZP_{ii'mt}$:becomes 1 if product i is after product i' on unit m at time period t, zero otherwise

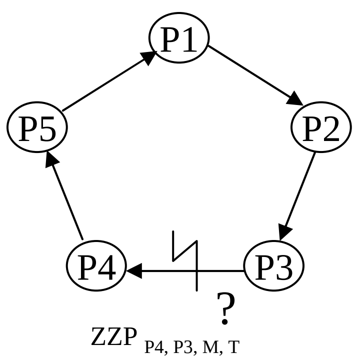
P1, P2, P3, P4, P5



2. **Break the cycle at the pair with the maximum transition time to obtain the sequence.**

KEY VARIABLE:

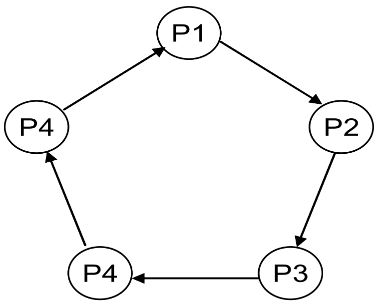
$ZZP_{ii'mt}$:becomes 1 if the link between products i and i' is to be broken, zero otherwise



=> P4→P5→P1→P2→P3

MILP Model

According to the location of the link to be broken:



P2, P3, P4, P5, P1 ⟶ $ZZP_{P1, P2, M, T} = 1$

P3, P4, P5, P1, P2 ⟶ $ZZP_{P2, P3, M, T} = 1$

P4, P5, P1, P2, P3 ⟶ $ZZP_{P3, P4, M, T} = 1$

P5, P1, P2, P3, P4 ⟶ $ZZP_{P4, P5, M, T} = 1$

P1, P2, P3, P4, P5 ⟶ $ZZP_{P5, P1, M, T} = 1$

The sequence with the <u>minimum total</u> transition time is the **optimal sequence** within time period t.

$$YP_{imt} = \sum_{i'} ZP_{ii'mt} \qquad \forall i, m, t$$

$$YP_{i'mt} = \sum_{i} ZP_{ii'mt} \qquad \forall i', m, t$$

$$YP_{imt} \wedge \left[\bigwedge_{i'\neq i} \neg YP_{i'mt}\right] \Leftrightarrow ZP_{iimt} \qquad \forall i, m, t$$

$$YP_{imt} \geq ZP_{i,i,m,t} \qquad \forall i, m, t$$

$$ZP_{i,i,m,t} + YP_{i',m,t} \leq 1 \qquad \forall i, i' \neq i, m, t$$

$$ZP_{i,i,m,t} \geq YP_{i,m,t} - \sum_{i'\neq i} YP_{i',m,t} \qquad \forall i, m, t$$

$$\sum_{i}\sum_{i'} ZZP_{ii'mt} = 1 \qquad \forall m, t$$

$$ZZP_{ii'mt} \leq ZP_{ii'mt} \qquad \forall i, i', m, t$$

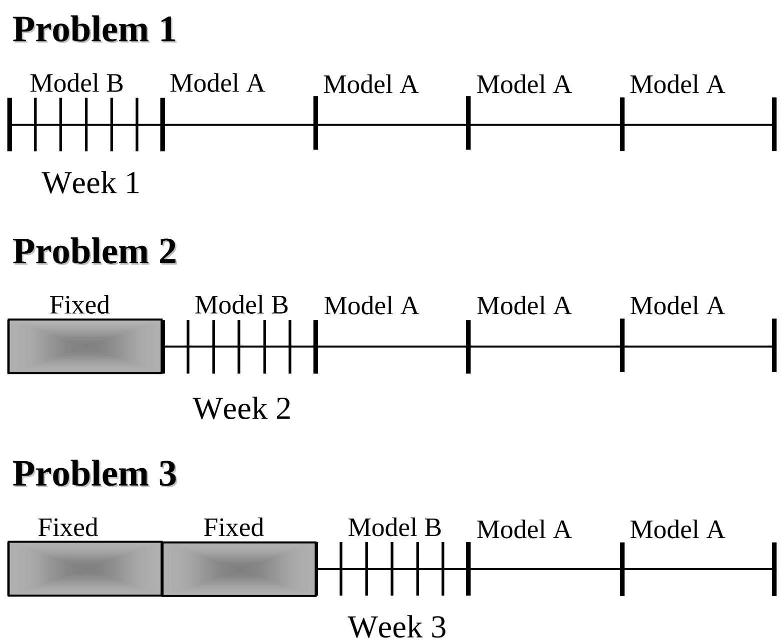
Generate the cycle and break the cycle to find the optimum sequence where transition times are minimized.

Having determining the sequence, we can determine **the total transition time** within each week.

Limitation: Large Problems

The **proposed planning models** may be expensive to solve for long term horizons.

ROLLING HORIZON APPROACH :



- ✓ The detailed planning period (Model B) moves as the model is solved in time.
- ✓ Future planning periods include only underestimations for transition times.

*Ref. Dimitriadis et al, 1997

EXAMPLE 1: 5 Products, 2 Reactors, 1 Week

	Method	Number of binary variables	Number of continuous variables	Number of Equations	Time (CPUs)	Solution ($)
A	Relaxed Planning	20	49	67	0.046	**1,680,960.0**
B	Detailed Planning	140	207	335	0.296	**1,571,960.0**
	Scheduling	594	2961	2537	150	**1,571,960.0**

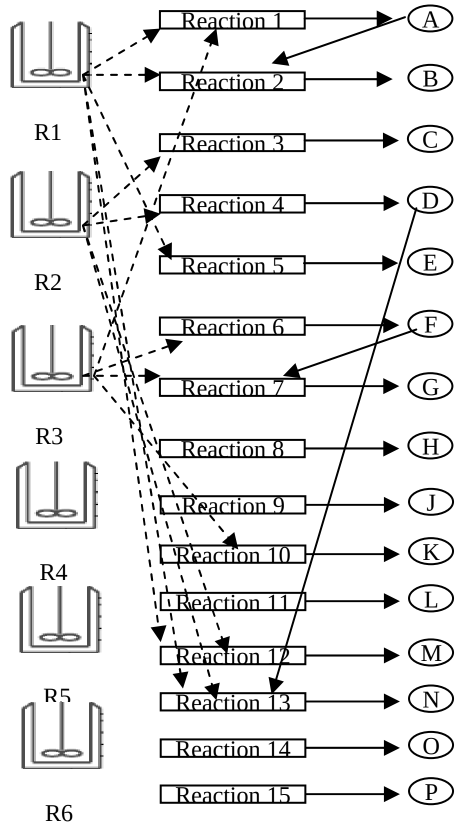
% 6.484 Difference

Obj Function Items ($)	Relaxed Planning	Detailed Planning	Scheduling
Sales	2,652,800	2,440,000	2,440,000
Operating Costs	971,840	868,000	868,000
Transition Costs	0	40	40
Inventory Costs	0	0	0

Detailed Planning and Scheduling are Identical!

EXAMPLE 2 - 15 Products, 6 Reactors, 48 Weeks

✓ **Determine the plan for 15 products, 6 reactors plant so as to maximize profit.**



- **15 Products, A,B,C,D,E,F,G,H,J,K,L,M,N,O,P**
- **B, G and N are produced in 2 stages.**
- **6 Reactors, R1,R2,R3,R4,R5,R6**
- **End time of the week is defined as due dates**
- **Demands are lower bounds**

Relaxed planning yields <u>21% overestimation of profit</u>

method	number of binary variables	number of continuous variables	number of equations	time (CPU s)	solution ($)
relaxed planning (A)	2,592	5,905	9,361	362	224,731,683
rolling horizon (RH)	10,092	25,798	28,171	11,656	184,765,965

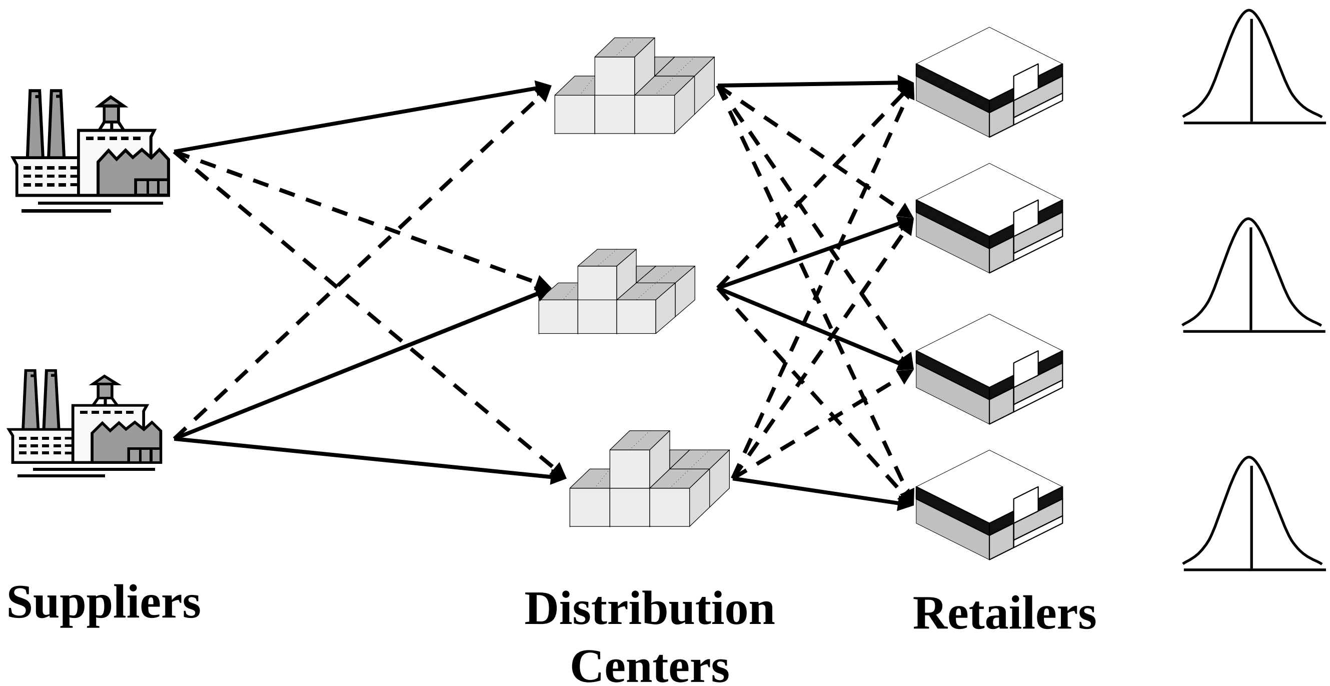
- ✓ **Inventory** is everywhere
- ✓ U.S. inventories*
  - ✓ Total value: $1.4 trillion (**≈** 10% U.S. GDP)
  - ✓ Estimated inefficiency: 50+ %
  - ✓ Economic opportunity: **$700+ billion**
- ✓ Gap in optimizing inventories across the entire Supply Chain
  - ✓ Which location to stock inventory? – Supply Chain Design
  - ✓ How much in each location under uncertainty? – Stochastic Inventory

(*U.S. Census Bureau, "Manufacturing and Trade Inventories and Sales in U.S.", October 2008; Smartops, S. Tayur, 2005)

Supply Chain Design with Stochastic Inventory Management

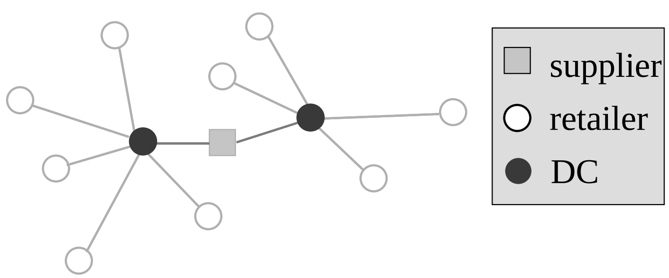
(Shen, Coullard, Daskin, 2003) *You, Grossmann (2008)*

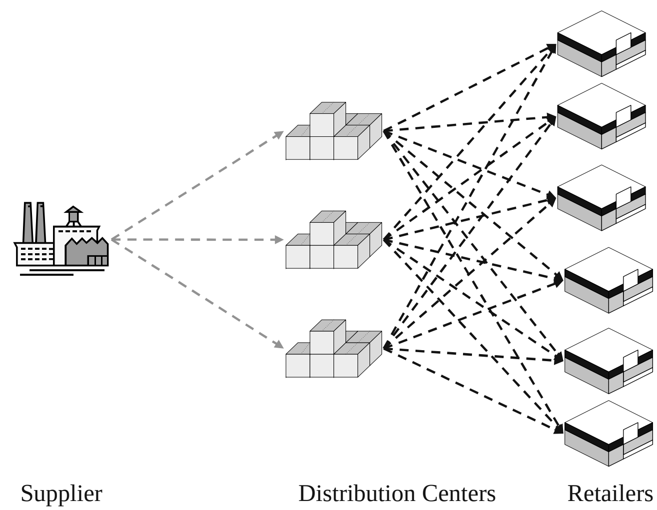
- Given: A potential supply chain
  - Including fixed suppliers, retailers and potential DC locations
  - Each retailer has uncertain demand, using (Q, r) policy
  - Assume all DCs have identical lead time L (lumped to one supplier)



Problem Statement

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





EOQ cost

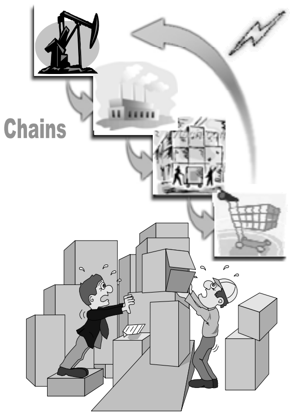
$$
\begin{aligned}
D &= \text{expected annual demand} = \sum \chi \mu_i Y_{ij} \\
v(x) &= \text{cost for shipping a order of size } x \text{ from supplier} \\
h &= \text{unit inventory holding cost} \\
F &= \text{fixed cost for place an order} \\
n &= \text{number of orders per year} \\
\chi &= \text{days per year} \\
L &= \text{order lead time} \\
\beta &= \text{weighted factor associated with the transportation cost} \\
\theta &= \text{weighted factor associated with the inventory cost}
\end{aligned}
$$

Annual EOQ cost at a DC:

$$F \cdot n + \beta \cdot n \cdot v(\frac{D}{n}) + \theta \cdot h \cdot \frac{D}{2n}$$

$v(x) = g + ax$

ordering cost | transportation cost | Working inventory cost



Working Inventory cost

Annual working inventory cost at a DC:

$$\underbrace{F \cdot n}_{\text{ordering cost}} + \underbrace{\beta \cdot n \cdot \left(g + \frac{aD}{n}\right)}_{\text{transportation cost}} + \underbrace{\theta \frac{h \cdot D}{2n}}_{\text{inventory cost}}$$

Convex Function of *n*

The optimal number of orders is:

$$n^* = \sqrt{((\theta hD)/2(F + \beta g))}$$

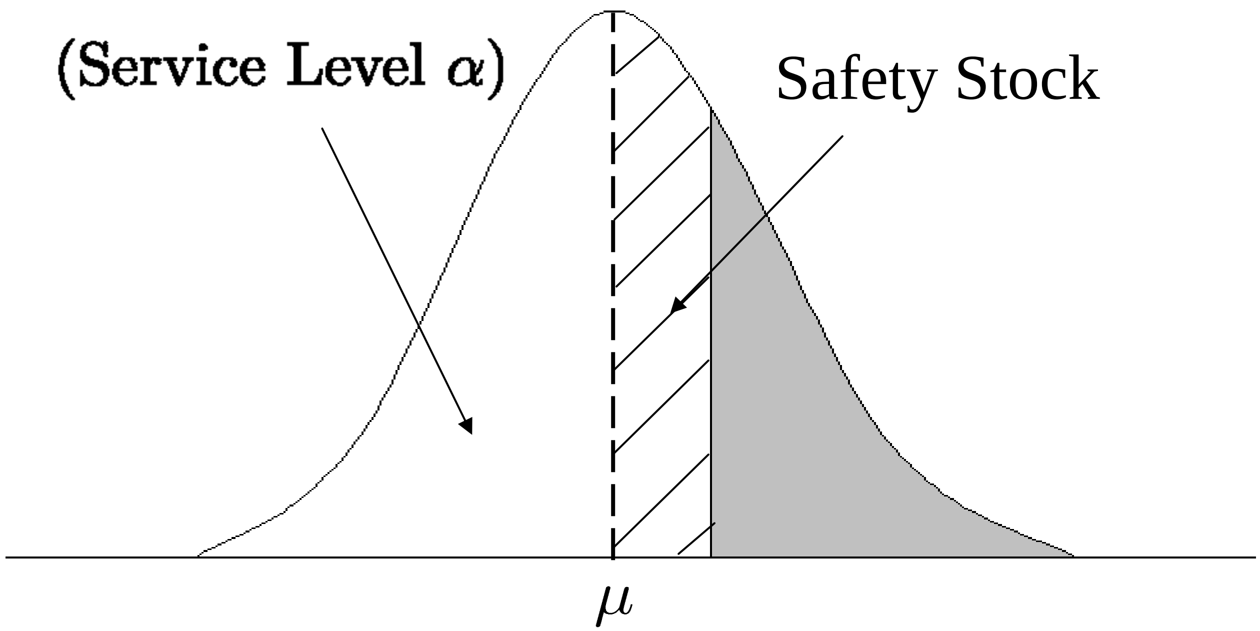
The optimal annual EOQ cost:

$$Fn + \beta v\left(\frac{D}{n}\right)n + \theta\frac{hD}{2n} = \boxed{\sqrt{2\theta hD(F + \beta g)} + \beta aD}$$

Safety Stock Level

$D \sim N(\mu, \sigma^2) \Longrightarrow$ Safety Stock = $\boxed{z_\alpha \sigma}$, $P(z \leq z_\alpha) = \alpha$ **(Service Level)**

Lead time = *L* $\Rightarrow D \sim N(L \cdot \mu, L \cdot \sigma^2) \Rightarrow$ $\boxed{\text{Safety Stock} = z_\alpha \sigma \sqrt{L}}$

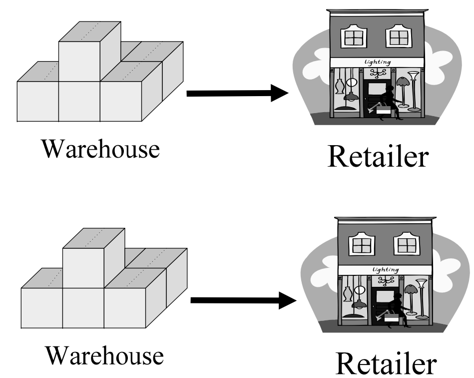


Risk-Pooling Effect*

- Single retailer: $$\text{safety stock} = z_\alpha \sigma$$

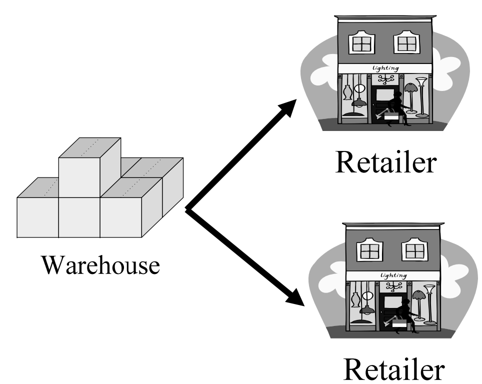
- Decentralized system:
  - Each retailer maintains its own inventory
  - Demand at each retailer: $D_i \sim N(\mu_i, \sigma_i^2)$

$$\text{safety stock} = z_\alpha \sum_{i=1}^{N} \sigma_i$$



- Centralized system:
  - All retailers share common inventory
  - Integrated demand: $\sum_i D_i \sim N(\sum_i \mu_i, \sum_i \sigma_i^2)$

$$\text{safety stock} = z_\alpha \sqrt{\sum_{i=1}^{N} \sigma_i^2}$$



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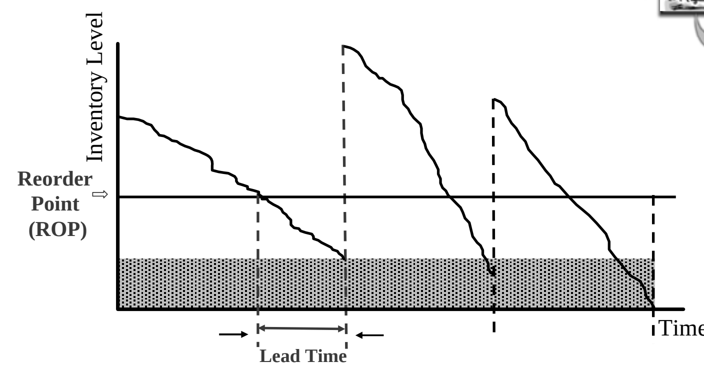
*** GD Eppen, "Effect of centralization in a multi-location newsboy problem", <u>Management Science</u>, 1979, 25(5), 498***

Safety Stock Cost for DCs

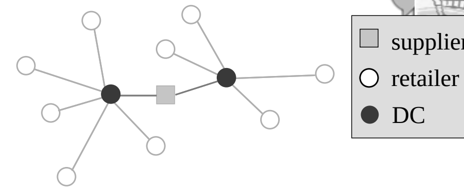


- Demand at retailer i ~ $N(m_i, s^2_i)$
- Centralized system (risk-pooling)
- Expected annual cost of safety stock at a DC is:

$$\text{safety stock cost} = \boxed{h \cdot z_\alpha \sqrt{L \sum_{i \in I} \sigma_i^2}}$$

where z_a is the standard normal deviate for which $P(z \leq z_\alpha) = \alpha$

Other Parameters and Variables



I *set of retailers indexed by I*

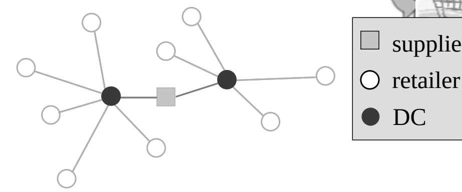
f_j *fixed (annual) cost for locating a DC j*

d_{ij} *shipping unit cost from DC j to retailer i*

$$X_j = \begin{cases} 1 & \text{if Distribution Center (DC) } j \text{ is selected} \\ 0 & \text{if not} \end{cases}$$

$$Y_{i,j} = \begin{cases} 1 & \text{if retailer } i \text{ is served by Distribution Center (DC) j} \\ 0 & \text{if not} \end{cases}$$

INLP Model Formulation



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

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

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

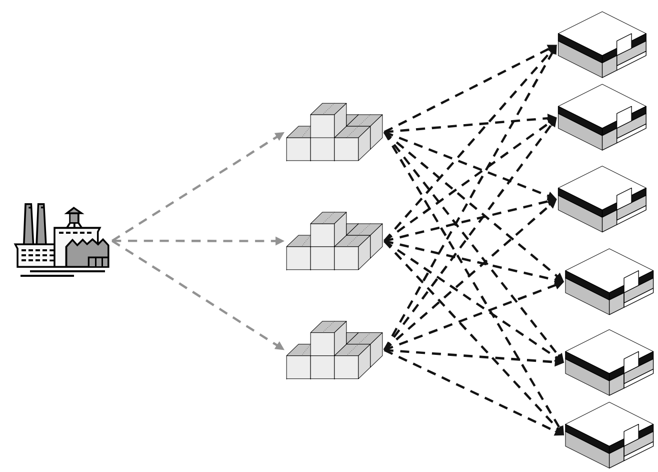
$$+ \quad \sum_{j\in J}(\theta h z_\alpha \sqrt{\sum_{i\in I}\sigma_i^2 L_i Y_{ij}})$$ Safety Stock

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

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

Assignments

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



Nonconvex INLP

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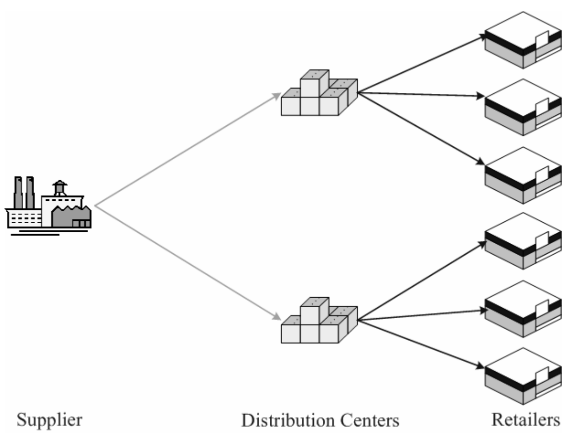
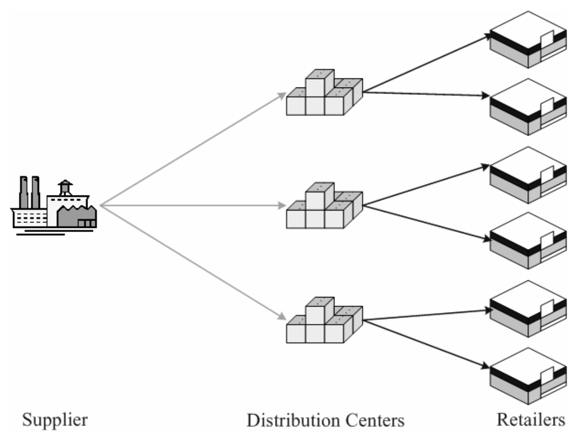
Illustrative Example

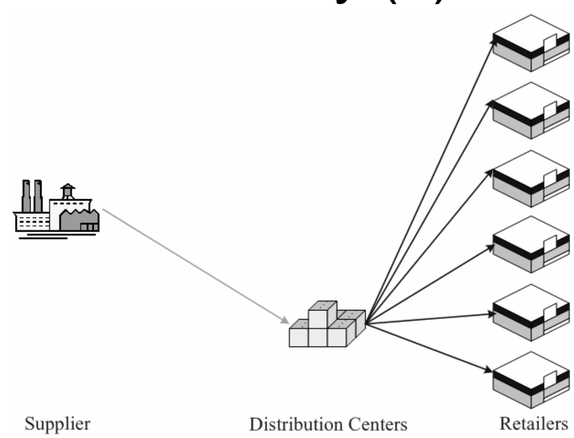
- Small Scale Example *(solved with BARON)*
  - A supply chain includes 3 potential DCs and 6 retailers (pervious slide)
  - Different weights for transportation (***β***) and inventory (***θ***)



β = 0.01, θ = 0.01



β = 0.1, θ = 0.01



β = 0.01, θ = 0.1

- Model Size for Large Scale Problem
  - INLP model for 150 potential DCs and 150 retailers has 22,650 binary variables and 22,650 constraints – need effective algorithm to solve it …

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)

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

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

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

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

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

Avoid unbounded gradient

Non-convex MINLP

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

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Lagrangean Relaxation

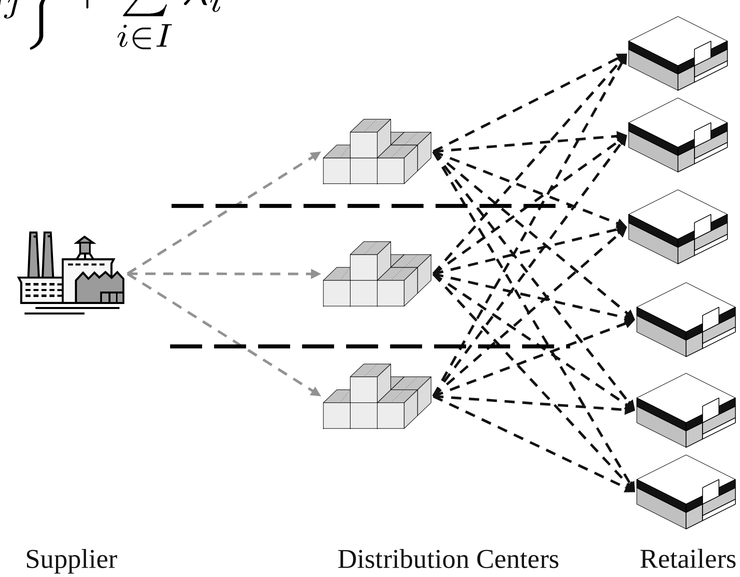
- Lagrangean Relaxation (LR) and Decomposition
  - LR: dualizing the single sourcing constraint: $\sum_{j \in J} Y_{ij} = 1, \forall i \in I$
  - Spatial Decomposition: decompose the problem for each potential DC *j*
  - Implicit constraint: at least one DC should be installed, $\sum_{j \in J} X_j \geq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

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

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

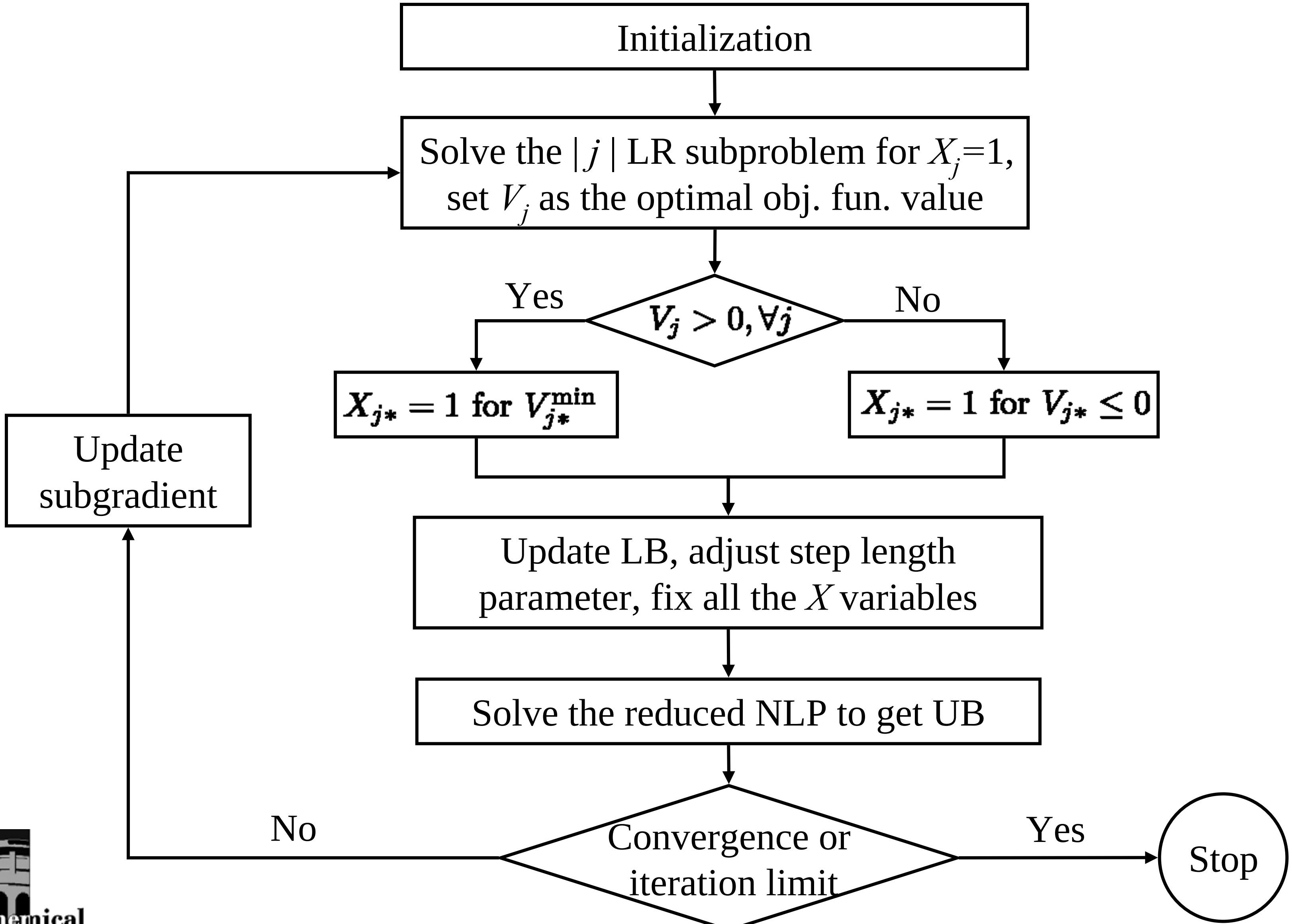
Concave

decompose by DC *j*



LR Algorithm Flowchart

Responsive Supply Chains



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Computational Results

- Case 2: 88 ~150 retailers
  - Each instance has the same number of potential DCs as the number of retailers

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 obtained with BARON for 10 hour limit.

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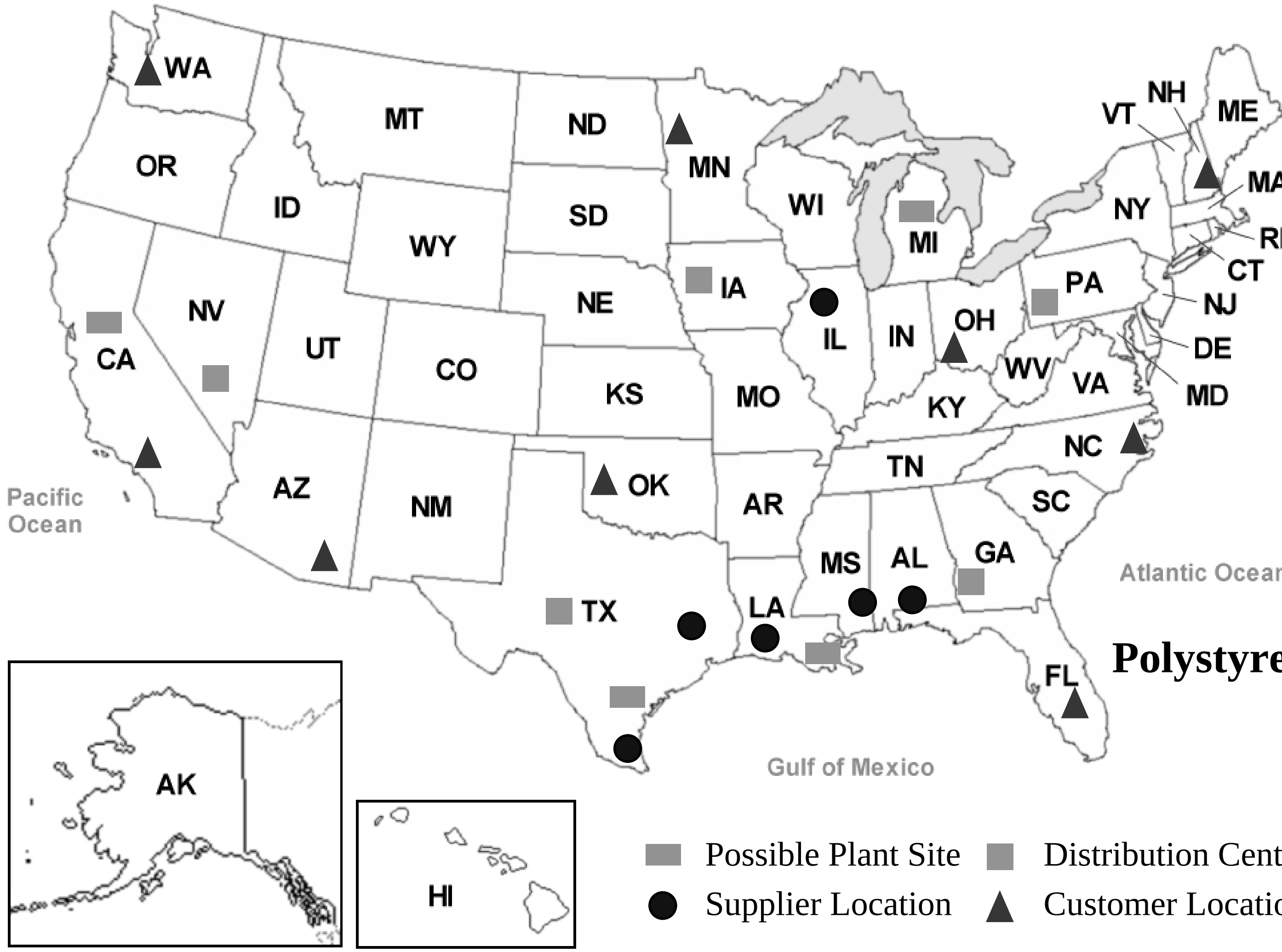
Optimal Design of Responsive Process Supply Chain

Responsive Supply Chains

You, Grossmann (2009)

Bicriterion MINLP
max NPV, max Responsiveness



Polystyrene Resins

Possible Plant Site   Distribution Center
Supplier Location   Customer Location

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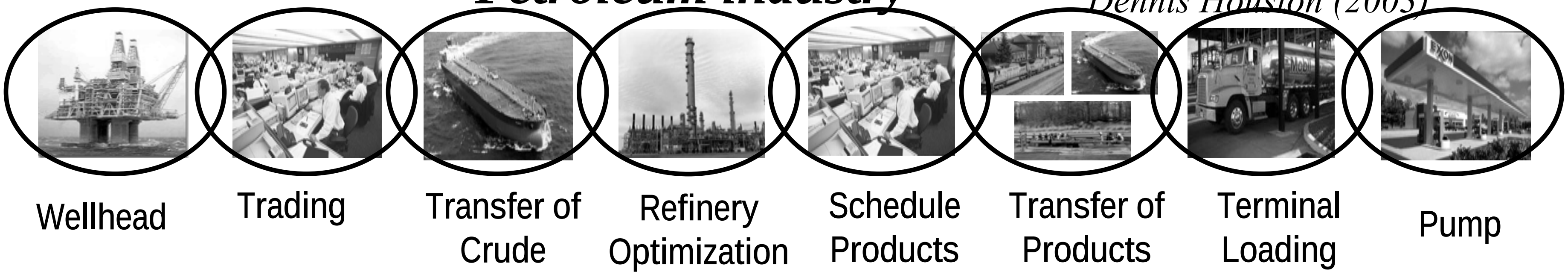
Source: Data Courtesy Nova Chemical Inc. *http://www.novachem.com/*

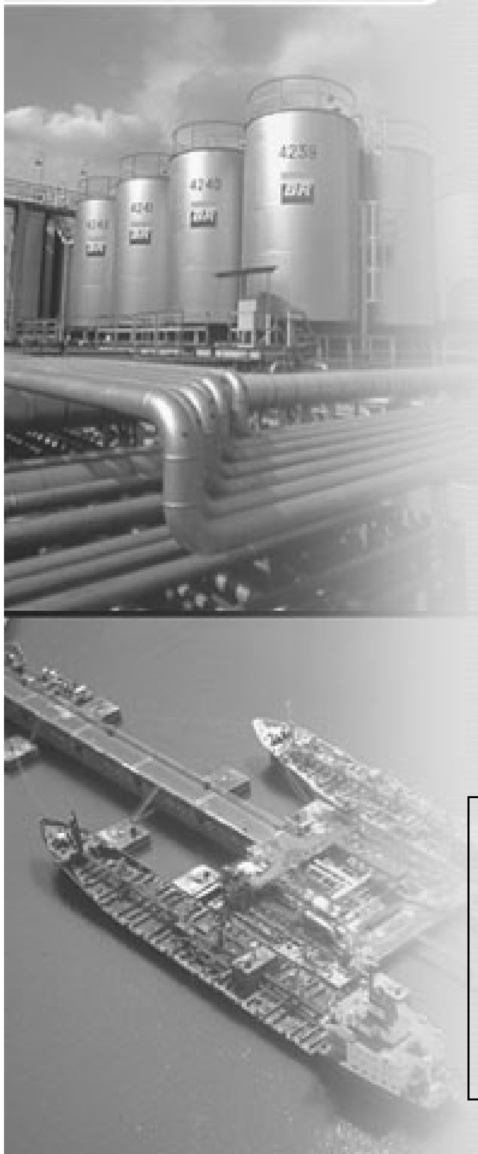
Petroleum industry

Dennis Houston (2003)

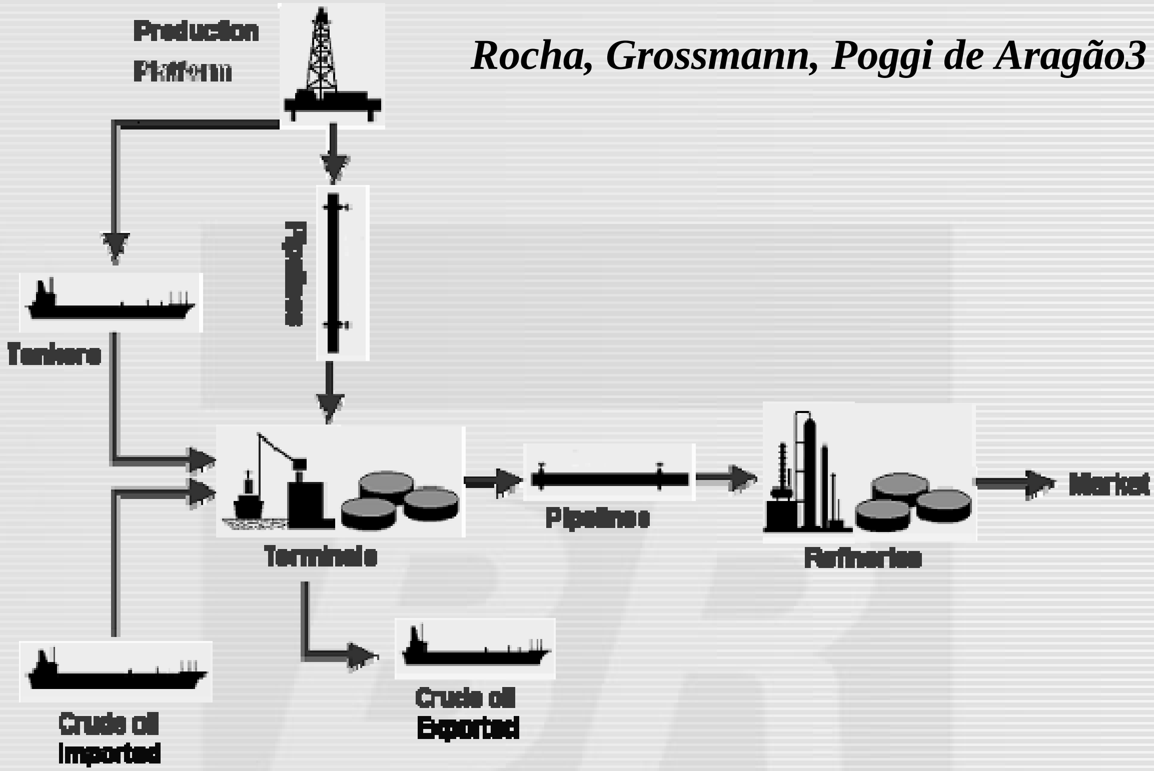


PETROBRAS

Petroleum Supply Chain Planning



Rocha, Grossmann, Poggi de Aragão3 (2009)



Decisions to be optimized:

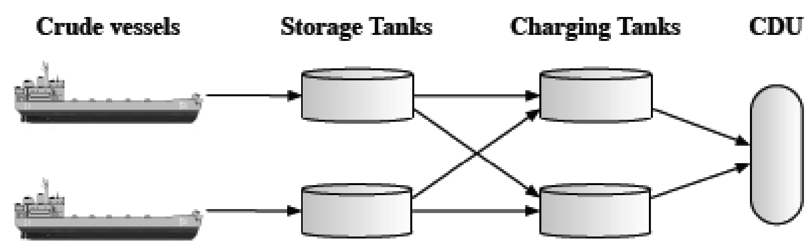
- When to offload platforms
- What class ship and volume
- Send to which terminal
- Final destination – which refinery

Very-large Scale MILP

Crude-oil operations scheduling problem

Mouret, Grossmann, Pestiaux (2009)

- Scheduling horizon $[0, H]$
- 4 types of resources:
  - Crude-oil marine vessels
  - Storage tanks
  - Charging tanks
  - Crude Distillation Units (CDUs)
- 3 types of operations:
  - Unloading: Vessel unloading to storage tanks
  - Transfer: Transfer from storage tanks to charging tanks
  - Distillation: Distillation of charging tanks

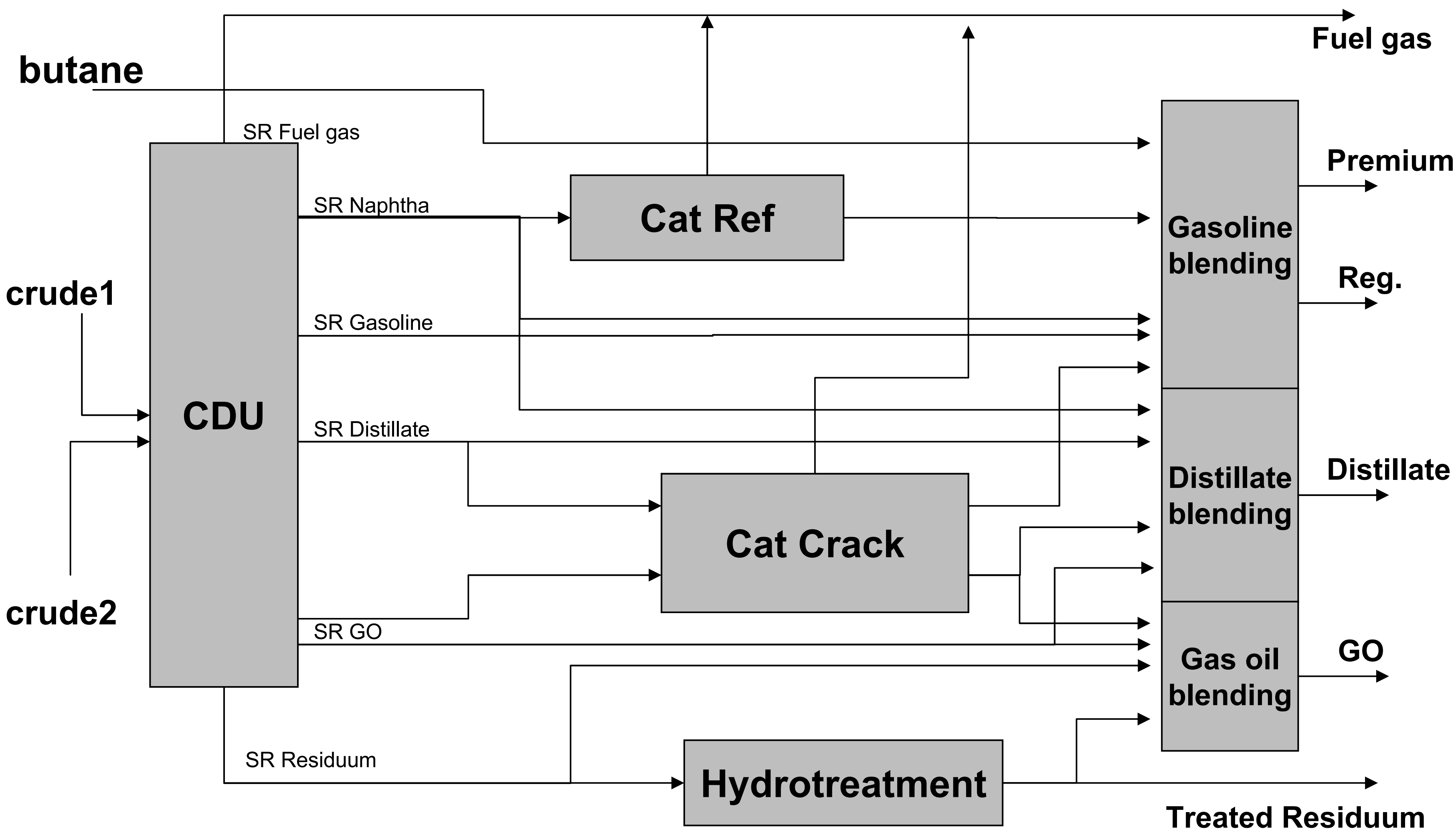


Global MINLP Optimization

Refinery Planning with Nonlinear Models

Alattas, Palou, Grossmann

Beyond PIMS *NLP model*



Optimal Development Planning under Uncertainty ExxonMobil

- **Simultaneously optimize the investment and operation decisions** ***Tarhan, Grossmann (2008)***
- **Offshore oilfield having several reservoirs under uncertainty**
- **For a project horizon of 10-30 years**
- **Maximize the expected net present value (ENPV) of the project**

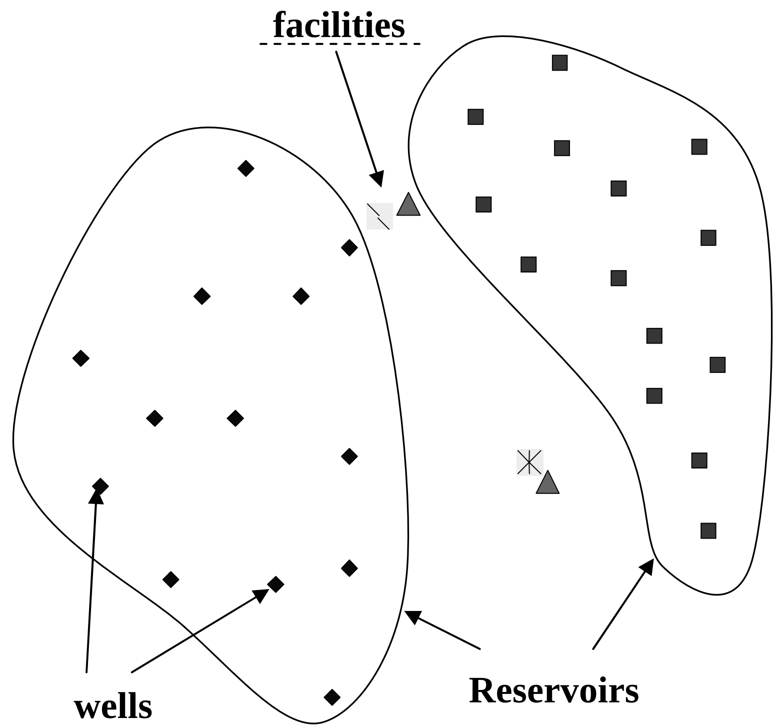
Decisions:

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

Uncertainty:

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

(endogenous)



Options for Infrastructure

ExxonMobil

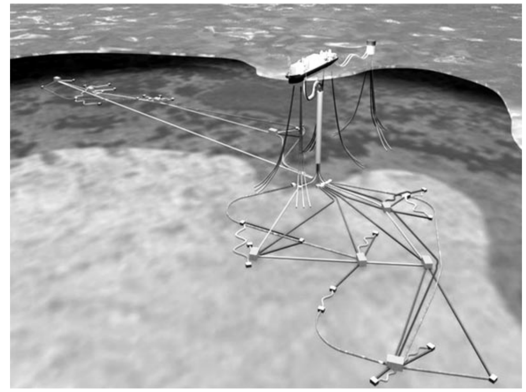
<u>FPSO:</u> (Floating Production Storage Offloading)

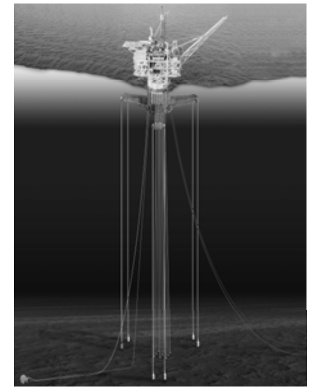
- **Small FPSO, converted from oil tanker**
  - **Low capacity**
  - **Less capital cost**
  - **Short construction time**

- **Large FPSO, grassroots facilities**
  - **High capacity**
  - **Higher capital cost (lower capex/capacity)**
  - **Long construction time**

<u>TLP:</u> (Tension-Leg Platform)

  - **Cannot process oil**
  - **Only drilling and oil recovering capability**





<u>Sub-sea well:</u>

- **Higher capital cost**
- **More flexible: can be drilled without any FPSO or TLP facility**
- **Connect to FPSO facility**

<u>TLP well:</u>

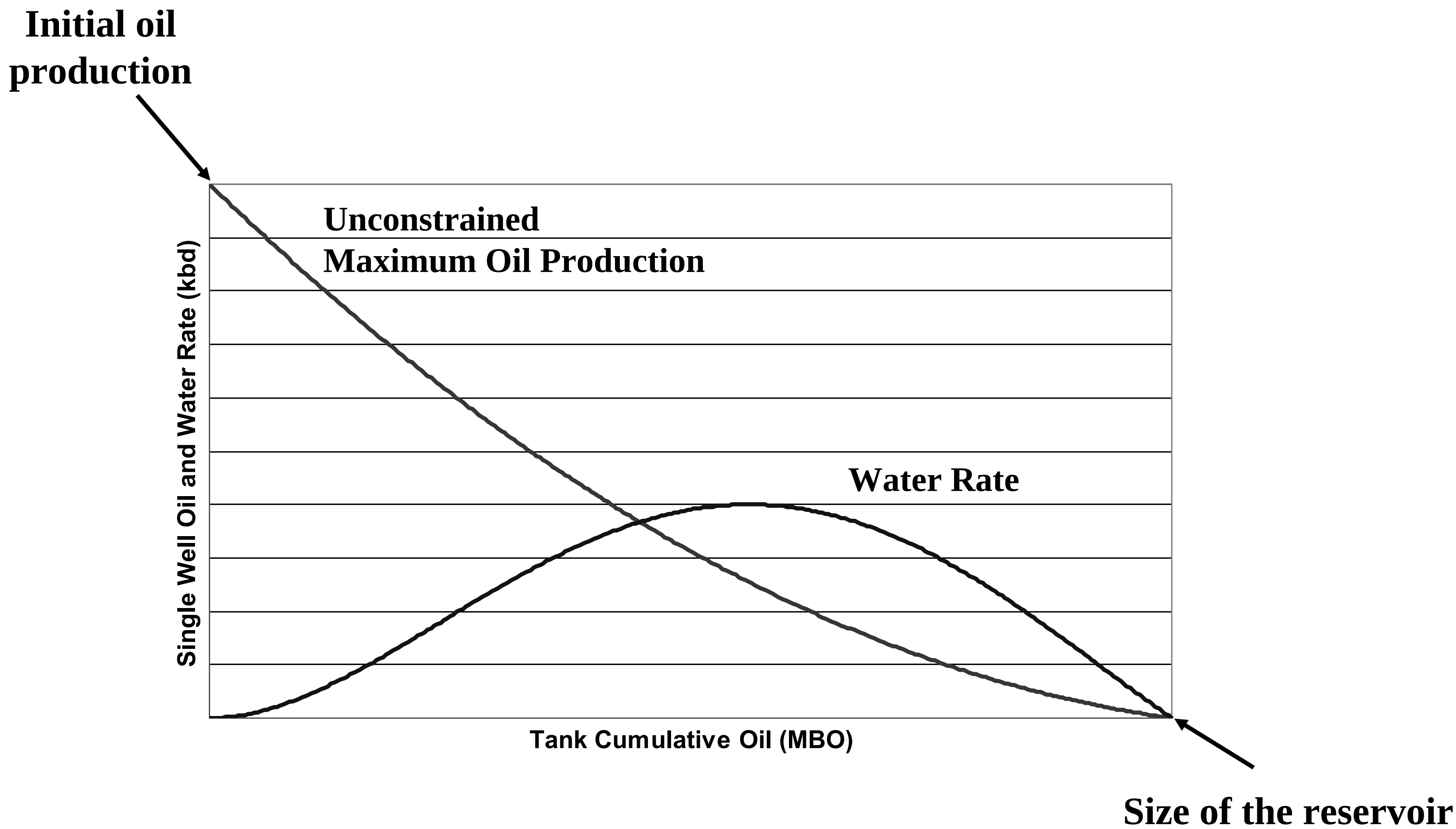
- **Less capital cost**
- **Less flexible: need TLP facility to drill**
- **Connect to TLP facility**

<u>Pictures taken from:</u>

(1) www.wikipedia.org (3) www.offshore-technology.com

(2) www.search.com (4) www.aas-jakobsen.no

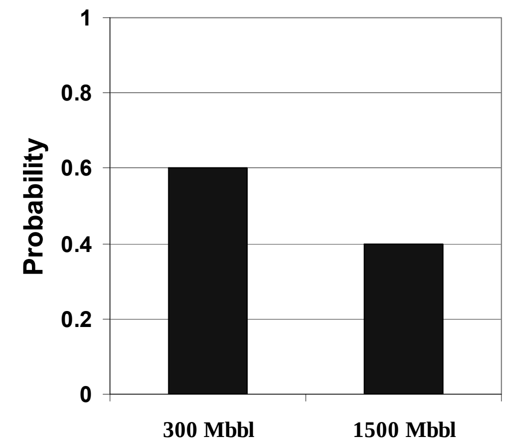
Non-linear Reservoir Model



Assumption: All wells in the same reservoir are identical.

Modeling Uncertainty Resolution Over Time

Uncertainty is represented by discrete probability distributions.



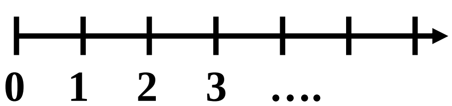
Gradual resolution:

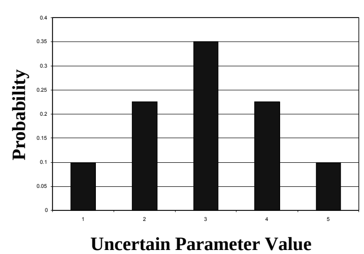
- Uncertainty in initial productivity resolves after
  drilling 3 wells (appraisal program)
  Note: Appraisal wells can be used for production.

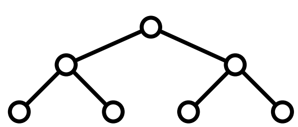
- Uncertainty in size of a reservoir resolves after
  drilling 9 wells **OR** producing oil for 1 year

- Uncertainty in water breakthrough time resolves after
  producing oil for 1 year

Discrete time horizon + Discrete distribution → Scenario trees



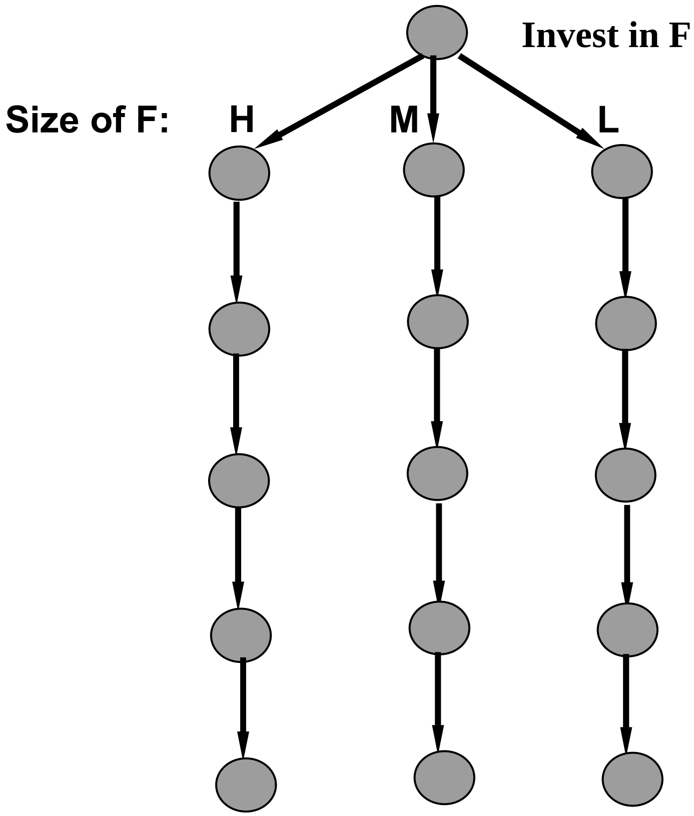




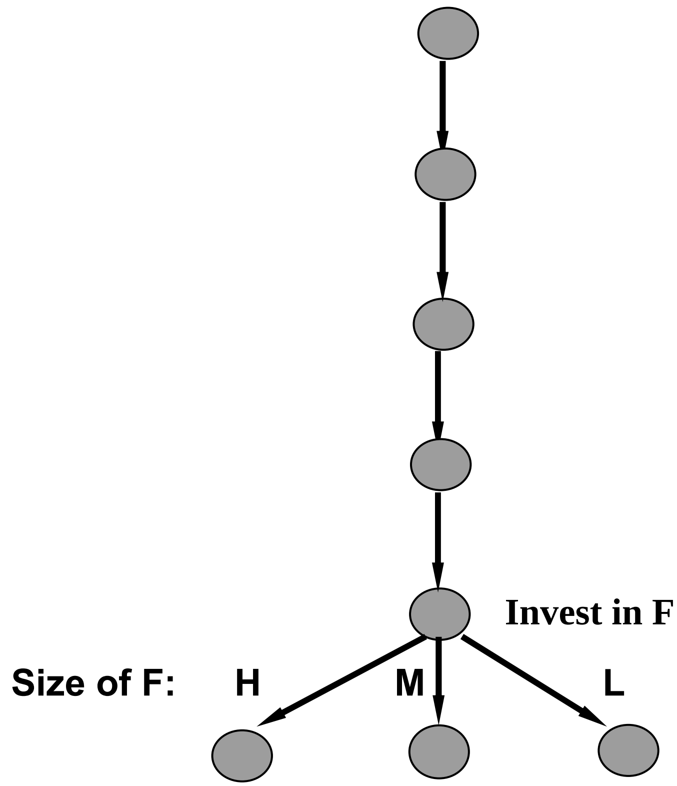
Decision Dependent Scenario Trees

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

Invest in F in year 1

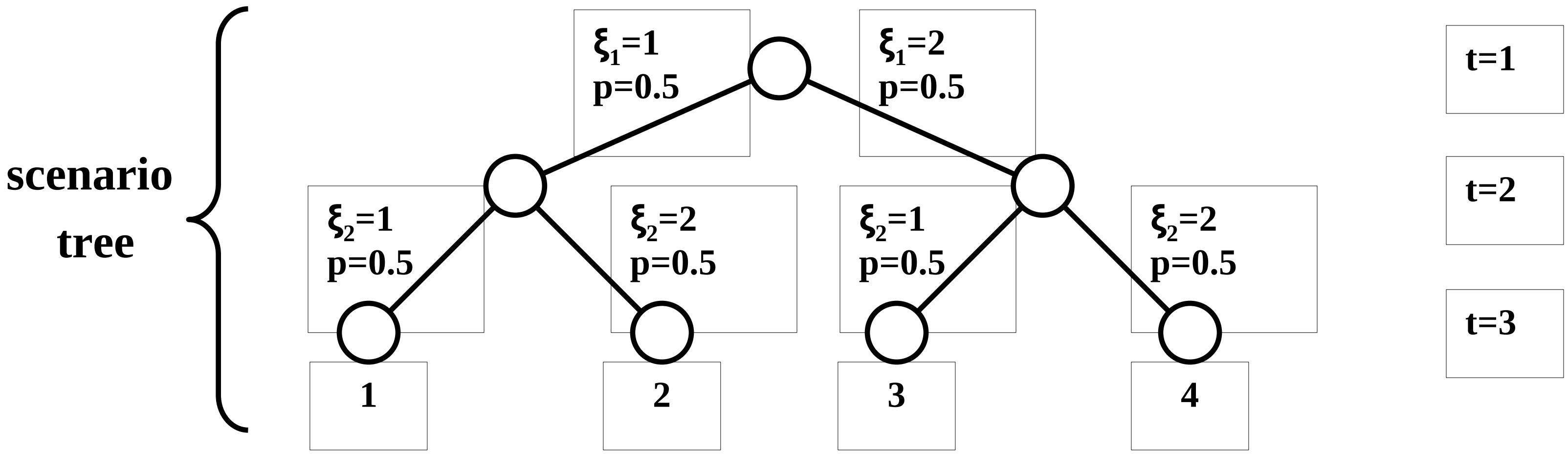


Invest in F in year 5

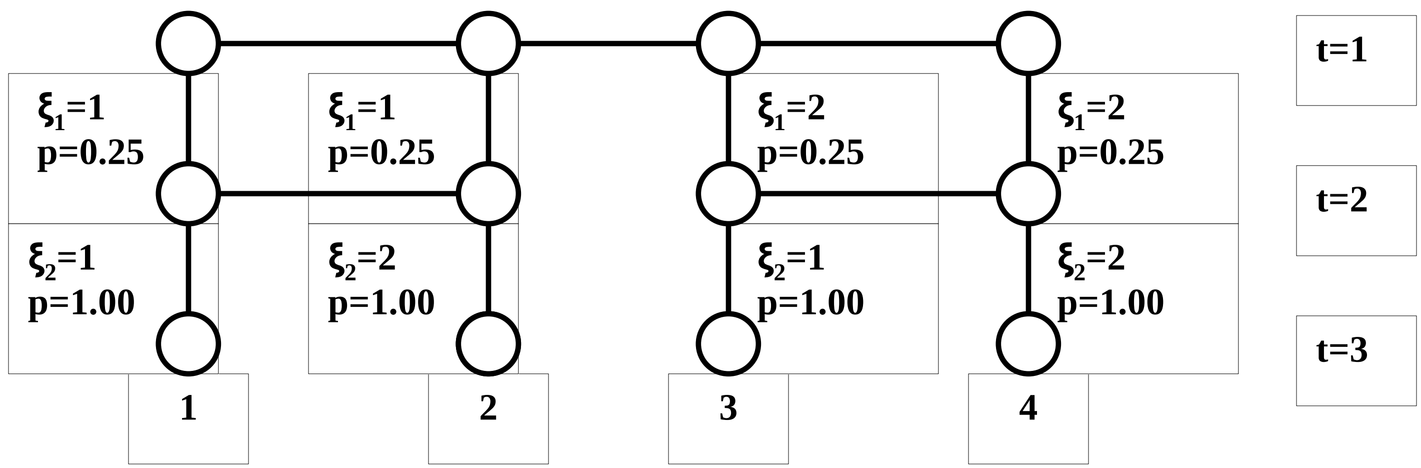


Scenario tree
- **Not unique: Depends on timing of investment at uncertain fields**
- **Central to defining a Stochastic Programming Model**

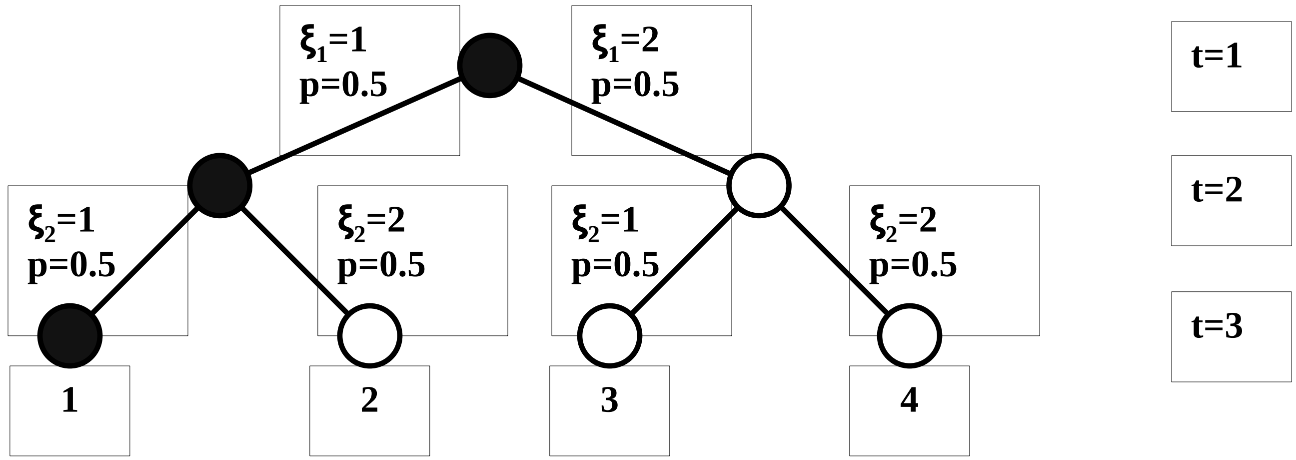
Stochastic Programming



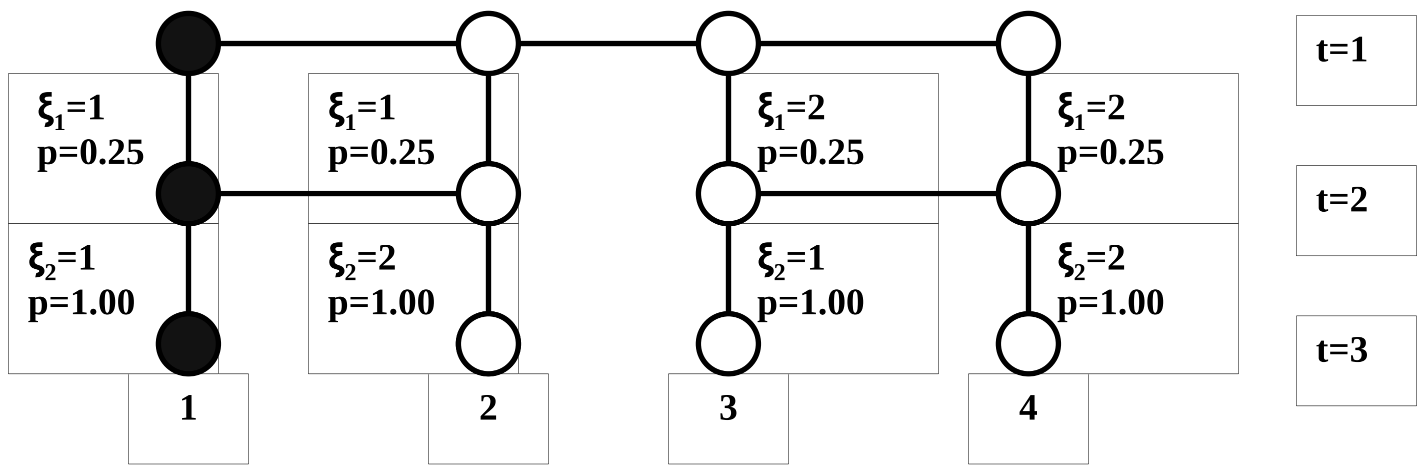
Alternative and equivalent scenario tree structure (Ruszczynski, 1997):



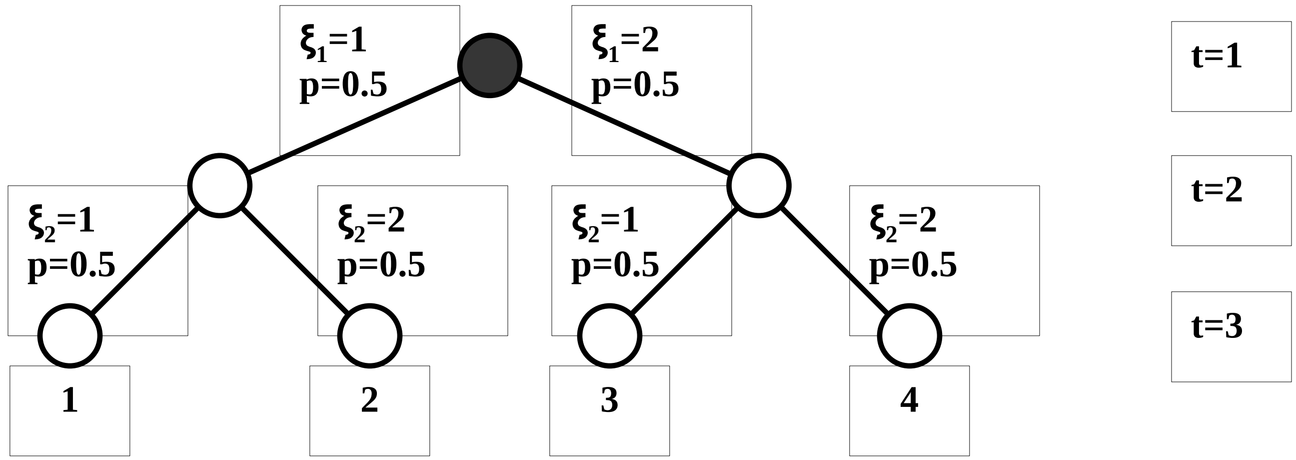
Stochastic Programming



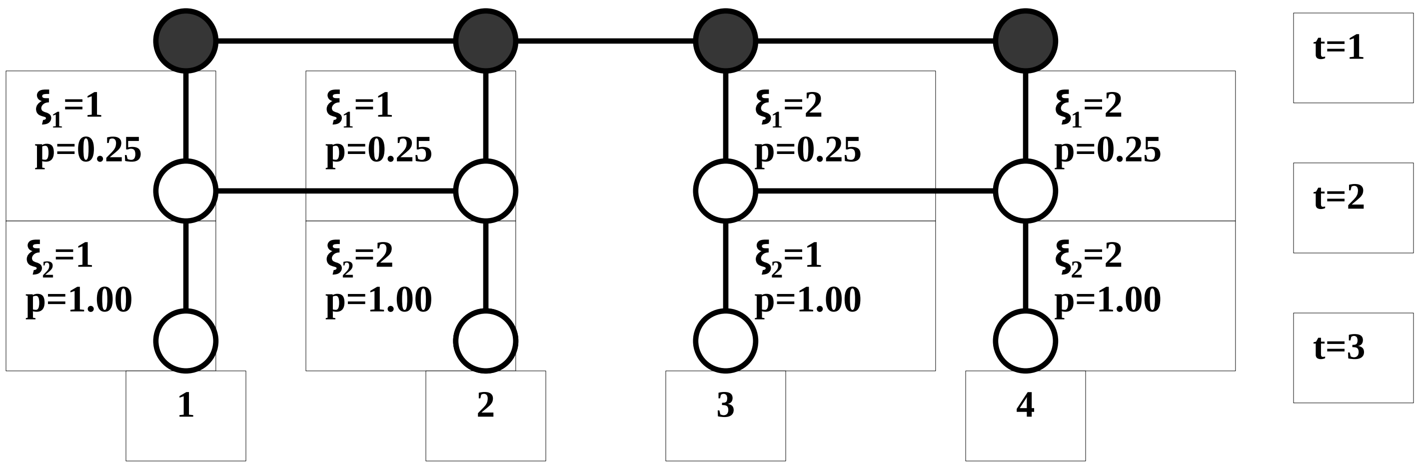
Each scenario is represented by a set of unique nodes



Stochastic Programming

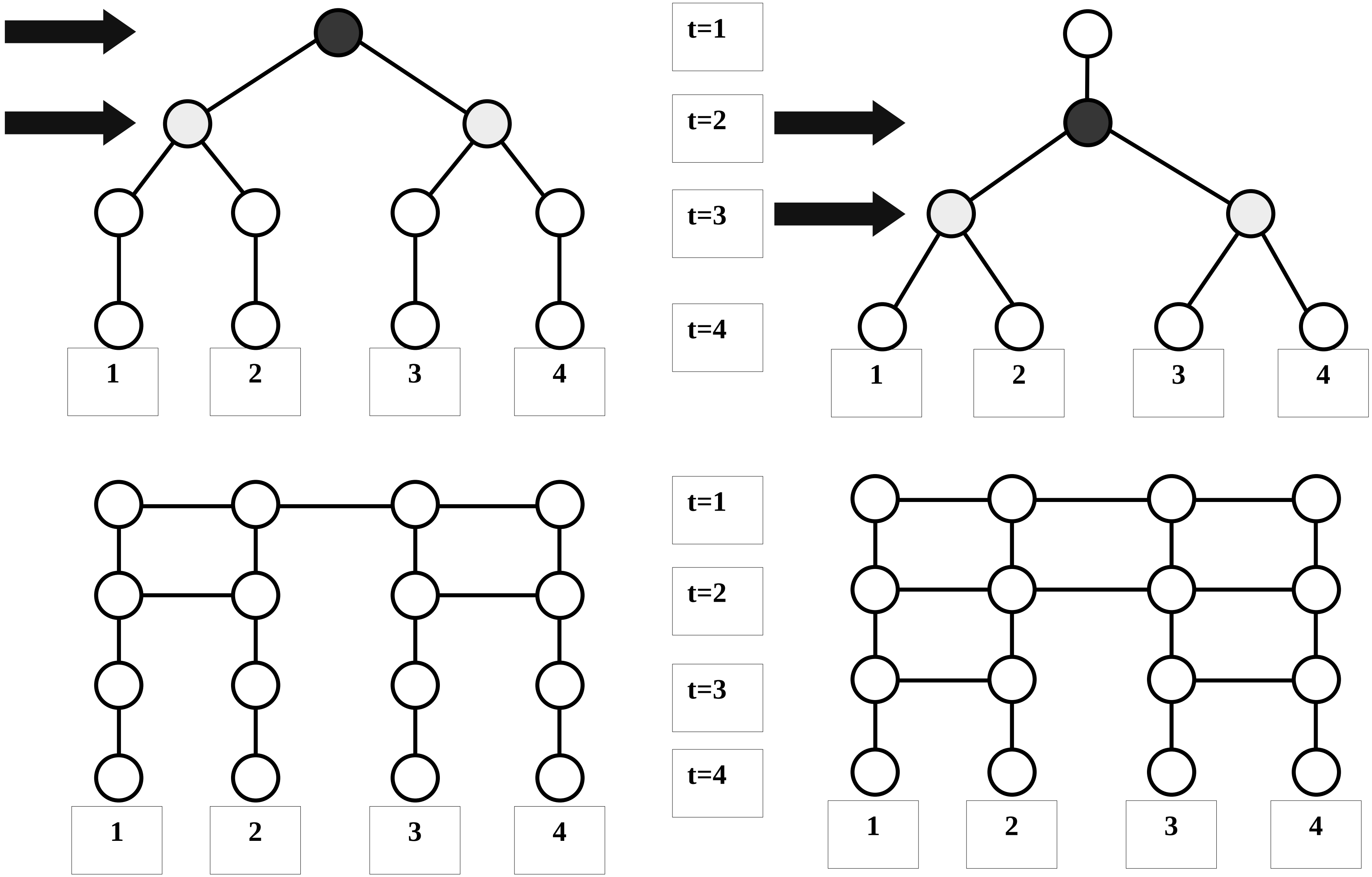


Nodes have same amount of information $\equiv$ Nodes are indistinguishable



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**

$$\mathrm{WOR} = a \times \left(\frac{\text{cumulative oil produced}}{\text{size of the reservoir}} \right)^{b}$$

- **Logic constraints relating decisions**

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

- **Non-anticipativity constraints**

For each scenario

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

Disjunctions (conditional constraints)

Problem size 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

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

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

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

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

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

Formulation of Lagrangean dual

Relaxation

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- **Penalty for equality constraints**

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

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

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

Model decomposes: one nonconvex MINLP for each scenario!

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

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

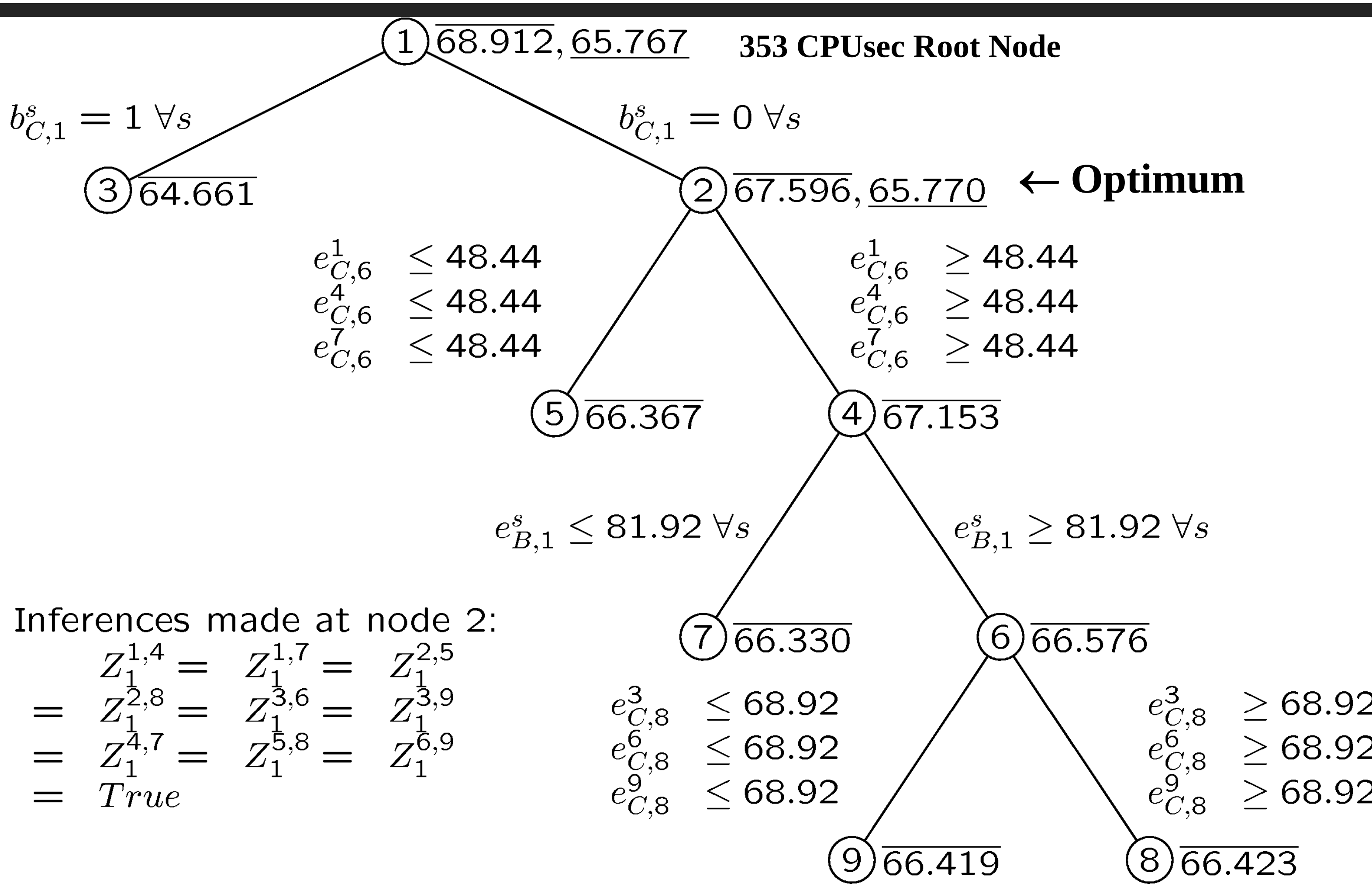
Lagrangean Relaxation: Upper bound for any λ

$$\sum_s \phi^s(\lambda) = \phi(\lambda) \ge \phi_{optimal} \quad \forall \lambda$$

Lagrangean Dual: Tightest upper bound

$$\phi_{LD} = \min_\lambda \phi(\lambda) \ge \phi_{optimal}$$

Example Branch and Bound Tree



9 nodes, 1683 CPU sec (1% optimality gap)

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

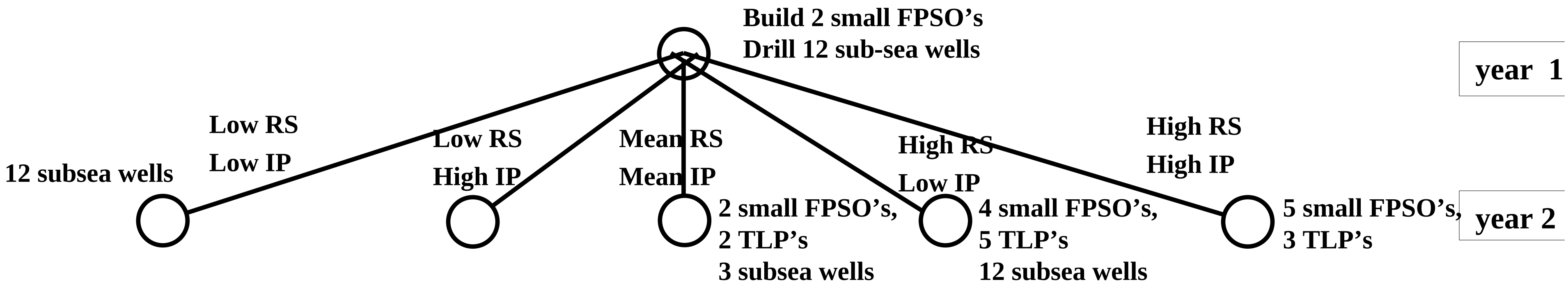
- **Wells are drilled in groups of 3.**
- **Maximum number of 12 sub-sea wells per year can be drilled.**
- **Maximum of 6 TLP wells per year per TLP facility can be drilled.**
- **Maximum of 30 TLP wells can be connected to a TLP facility.**

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

Stochastic Programming Approach

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

E[NPV] = $\$4.92 \times 10^9$



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.

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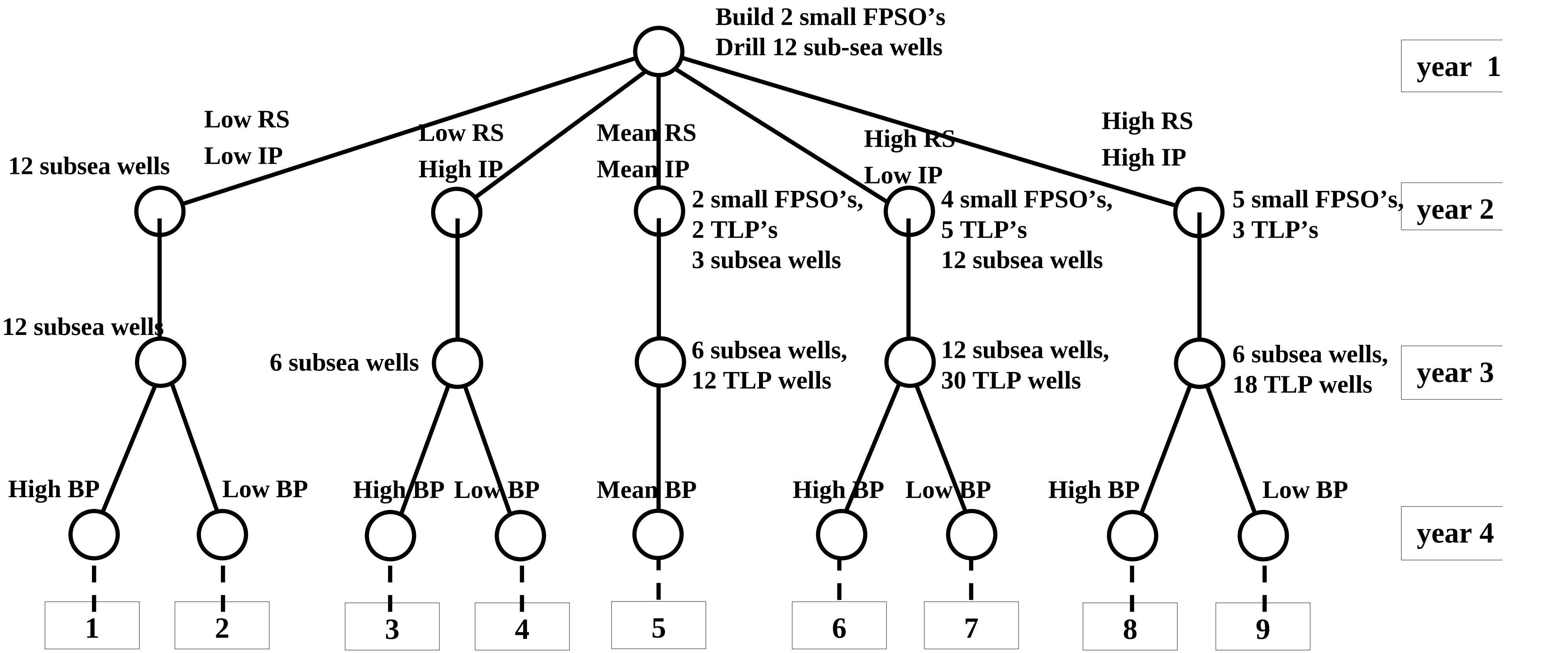
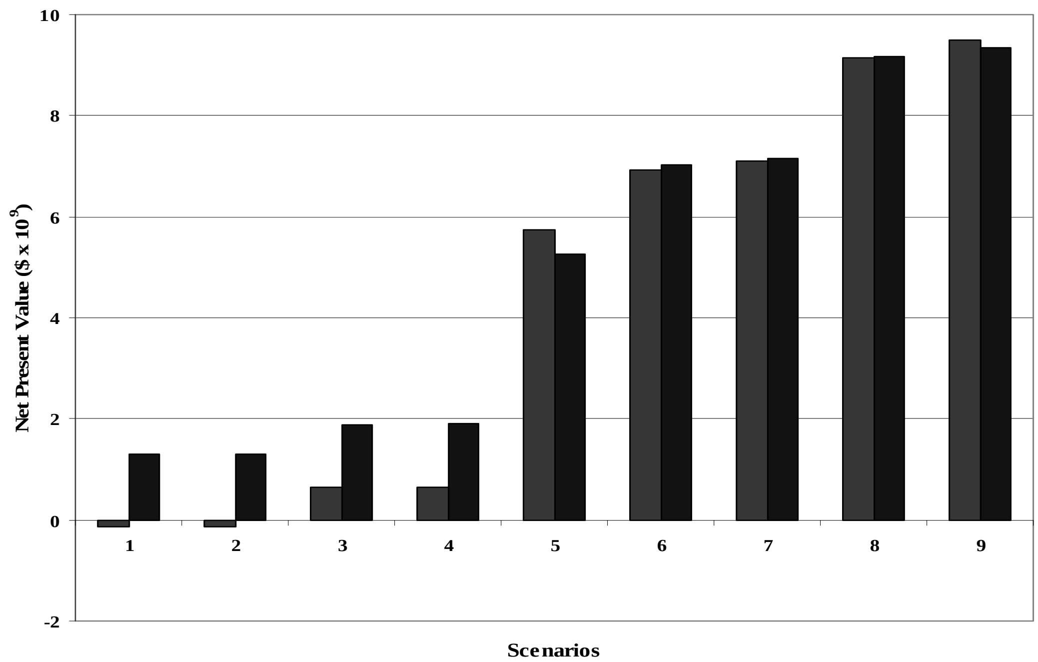


Solution proposes building 2 small FPSO's in the first year and then add new facilities / drill wells (recourse action) depending on the positive or negative outcomes.

Distribution of Net Present Value



Mean Value = $4.38 x 10^9

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

Conclusions

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

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)