Opening Remarks

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University of Oklahoma (OU) and State University of Rio de Janeiro (UERJ)

Active Informal Partnerships with:

- Eduardo Mach Queiroz: Federal University of Rio de Janeiro
- Argimiro Resende Secchi: Federal University of Rio de Janeiro
- Carlos Fischer: Institute for Development and Design. Argentina
- Diego Oliva: Institute for Development and Design. Argentina
- Pio Aguirre: Institute for Development and Design. Argentina
- Zuwei Liao: Zhejiang University. Hangzhou, China. (Post Doc. Chenglin Chang, Student Qucheng Lin)
- Sung Young Kim: Kyung Hee University, Korea
- Esdras Carvalho: State University of Maringá, Brazil
- Mauro Ravagnani: State University of Maringá, Brazil (Student Carolina Borges de Carvalho)
- Rohit Singla. Thapar Institute of Engineering and Technology. India

Main Research Goals

Use of GLOBAL Optimization for:

- The design of chemical and continuous manufacturing processes equipment.
    - **Heat Exchangers (S&T, Plate, Double Pipe, etc.)**
    - **Distillation Columns & Flash Separation Units, Absorbers, Strippers**
    - **Reactors**
    - **Fired Heaters**
- Simultaneous design of multiple equipment
    - **Cooling Water Systems**
    - **Train of Heat Exchangers**
- The synthesis of Heat Exchanger Networks (HEN)
- The synthesis of Work & Heat Exchanger Networks (WHEN)
- The synthesis of Entire Flowsheets

Main Technology Transfer Goals

Provide TOOLS to INDUSTRY for the optimal design of :

- Processes equipment (Heat Exchangers, Distillation & Absorption Columns, Reactors, etc.)
- Energy recovery (HEN & WHEN)
- Entire flowsheets including HEN/WHEN, separation processes and reactors.

Use contributing funds for

- Scholarships & Supporting personnel compensation
- Travel expenses
- Consortium professional and support activities

Main Technology Transfer Mechanisms

We envision the formation of an INDUSTRIAL/ACADEMIC CONSORTIUM.

with similar in structure as

- Center for Advanced Process Decision-making (CAPD)
  http://capd.cheme.cmu.edu/
- INSTITUT FRANCAIS DU PETROLE (IFP)
  https://www.ifpenergiesnouvelles.com/

MAIN RESEARCH FEATURES

We aim at producing technology that is:

- Directly Applicable and Usable in the Process Industry via appropriate graphical interfaces.
- Minimizing Cost (Total annualized) or Maximizing Profit (when investment is involved)
- Guaranteed Globally Optimal Answers
- Robust, without convergence problems
- Handling Uncertainty and Managing Financial Risk

MAIN RESEARCH TRAITS

We are currently exploring:

- Departure from the use of heuristic-based “Trial and Verification” procedures
- New Mathematical Programming Approaches
- Departures from Mathematical Programming to the use of Set Trimming and Enumeration Techniques
- Use of more rigorous models instead of analytical simplified models
- Use of Parallel Computing with the possible aid of Supercomputers
- Handling Uncertainty and Financial Risk

MAIN RESEARCH TRAITS

An overview about some of these ideas were discussed here:

I&EC research
Industrial & Engineering Chemistry Research

Article

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110th Anniversary: On the Departure from Heuristics and Simplified Models toward Globally Optimal Design of Process Equipment

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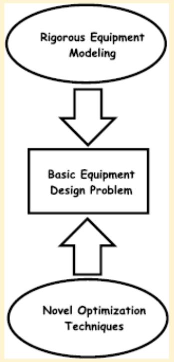
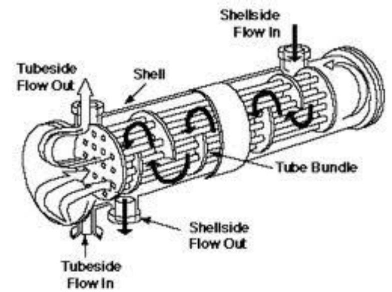
ABSTRACT: Despite the large advances in computational tools attained by the Process Systems Engineering community, industry for the most part still performs basic design of process equipment using trial-and-verification procedures guided by heuristic rules. In this opinion article, we present a discussion on how to depart from the use of these heuristics-based procedures, most step-by-step, sometimes computer-aided. We believe that there are direction changes, some incipient and some in full development already, toward the use of optimization tools for the task. The academic literature is dominated by mixed-integer nonlinear models, solved using different techniques (mostly stochastic or mathematical programming-based). These procedures have practical limitations that have hindered the migration of practitioners away from current heuristics and simplified model-based tools. We discuss these drawbacks and propose solutions. We first show how the use of commercially available discrete values of the design geometrical variables followed by reformulation can render linear models, solved using mixed-integer linear programming, sometimes integer linear programming. We also show how reformulation or judicious discretization of continuous



DEPARTURE FROM HEURISTICS

- Heuristics are based on “trial and verification” using Rules of Thumb
  - Used for HEX, Distillation Trays, Flash separation, etc.
  - Example:



1) Propose a heat exchanger type
2) Propose a value of U and obtain Area
3) Propose Shell & tubes D, Length, baffles, # passes
4) Check if the design is acceptable ($U_{calc}>U_{assumed}$)
5) If the solution is OK, stop
6) Otherwise, propose modifications (step 3 or step 2) (How, is not clear)

- This procedure DOES NOT guarantee optimality, not even local
- We are working to propose alternatives to each of these

NEW MATHEMATICAL PROGRAMMING APPROACHES

Our main approach is:

- Start with Mixed Integer Nonlinear Models (MINLM)
- Propose to solve them globally by adding an Objective (Area, Cost, etc)
- We incorporate discrete representations of geometry (standard values)
- We follow by reformulation and rigorous linearization
- The resultant formulation is linear: no convergence problems, no chance to be trapped in a poor local optimum when using Mathematical programming to solve the optimization

NEW MATHEMATICAL PROGRAMMING APPROACHES

Reformulation: Typical tube-side heat transfer coefficient

$$ht = \frac{0.023\, Ret^{0.8}\, \widehat{Prt}^{n}\, \widehat{kt}}{dti}$$ Heat transfer coefficient

$$Ret = \frac{dti\; v\; \widehat{\rho t}}{\widehat{\mu t}} = \frac{4\; \widehat{mt}}{Ntt\; \pi\; \widehat{\mu t}\; dti}$$ Reynolds number

We write

$$dti = \sum_{sd=1}^{sdmax} \widehat{pdti}_{sd}\; yd_{sd} \qquad \sum_{sdmin}^{sdmax} yd_{sd} = 1$$ Diameter in terms of discrete options

$$Ntt = \sum_{sd=1}^{sdmax} \widehat{pNtt}_{sNtt}\; yNtt_{sNtt} \qquad \sum_{sNttmin}^{sNttmax} yNtt_{sNtt} = 1$$ Number of tubes is discrete

NEW MATHEMATICAL PROGRAMMING APPROACHES

Reformulation of summation terms

$$ht = \frac{0.023\, Ret^{0.8}\, \widehat{Prt}^{n}\, \widehat{kt}}{dti}$$

$$ht = \frac{0.023\widehat{Prt}^{n}\, \widehat{kt}}{\left(\sum_{sdmin}^{sdmax} \widehat{pdti}_{sd}\, yd_{sd}\right)^{1.8}} \left(\frac{4\widehat{mt}}{\pi\widehat{\mu t}\sum_{sd=1}^{sdmax} \widehat{pNtt}_{sNtt}\, yNtt_{sNtt}}\right)^{0.8}$$

This is the key step

$$ht = 0.023\, \widehat{Prt}^{n}\, \widehat{kt}\left[\frac{4\,\widehat{mt}}{\pi\,\widehat{\mu t}}\right]^{0.8} \sum_{sd=1}^{sdmax}\sum_{sNtt=1}^{sNttmax} \frac{yNtt_{sNtt}\, yd_{sd}}{\widehat{pdti}_{sd}^{\;1.8}\, \widehat{pNtt}_{sNtt}^{\;0.8}}$$

NEW MATHEMATICAL PROGRAMMING APPROACHES

Strict Rigorouos Linearization

$$ht = 0.023\,\widehat{Prt}^{n}\,\widehat{kt}\left[\frac{4\,\widehat{mt}}{\pi\,\hat{\mu}}\right]^{0.8}\sum_{sd=1}^{sdmax}\sum_{sNtt=1}^{sNttmax}\frac{yNtt_{sNtt}yd_{sd}}{\widehat{pdti}_{sd}^{\;1.8}\,\widehat{pNtt}_{sNtt}^{\;0.8}}$$

$$\Rightarrow \begin{cases} ht = 0.023\,\widehat{Prt}^{n}\,\widehat{kt}\left[\frac{4\,\widehat{mt}}{\pi\,\hat{\mu}}\right]^{0.8}\sum_{sd=1}^{sdmax}\sum_{sNtt=1}^{sNttmax}\frac{wyNttd_{sNtt,sd}}{\widehat{pdti}_{sd}^{\;1.8}\,\widehat{pNtt}_{sNtt}^{\;0.8}} \\ wyNttd_{sNtt,sd} \le yNtt_{sNtt} \\ wyNttd_{sNtt,sd} \le ydt_{sd} \\ wyNttd_{sNtt,sd} \ge ydt_{sd} + yNtt_{sNtt} - 1 \end{cases}$$

RESULTING IN a Mixed Integer Linear Model (MILM)

NEW MATHEMATICAL PROGRAMMING APPROACHES

This approach rendered several articles

- Shell & Tube HEX Kern Method (ILP) (Carolina Gonçalves UERJ)
- Shell & Tube HEX Bell Delaware Method (MILP)) (Carolina Gonçalves, UERJ)
- Shell & Tube HEX as above with fouling modeling (MILP) (Julia Lemos, UERJ)
- Plate exchangers Double Pipe exchangers (MILP) (Natalia Martins, Andre Nahes, UERJ)
- Condensers (MILP) (João Domingues, UERJ) (Zuwei Liao, Zhejiang U.)
- Flash Separation units (MILP) (Carlos Fischer, Ingar)

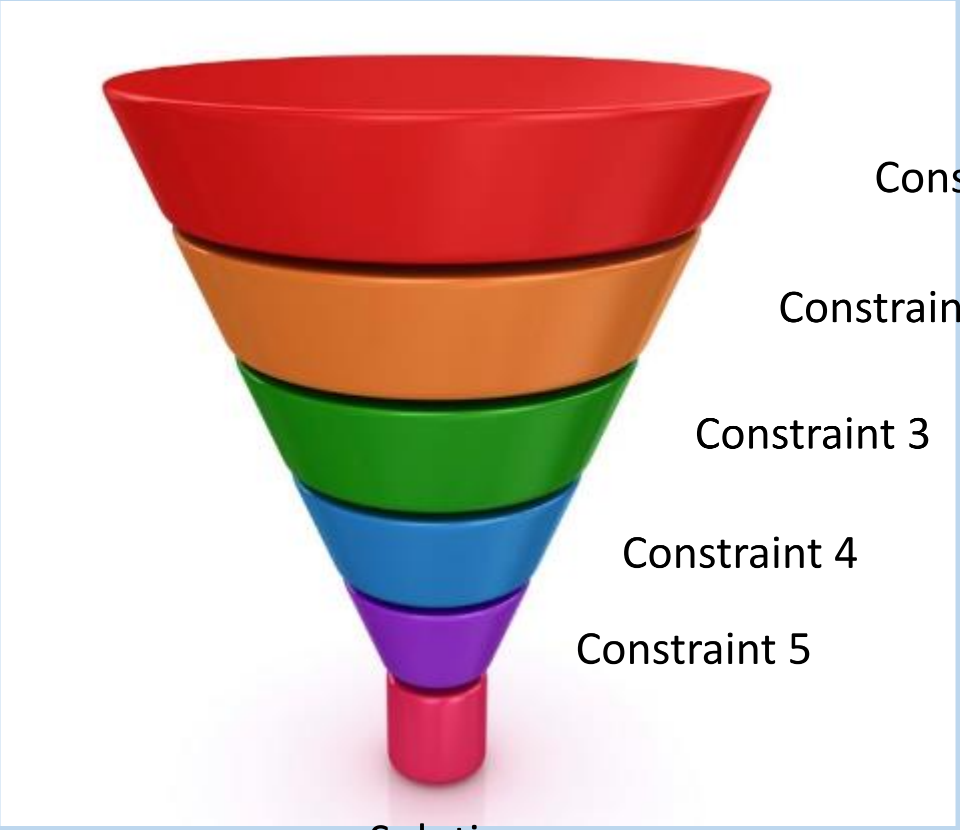
DEPARTURE FROM MATHEMATICAL PROGRAMMING

We also proposed to reduce the search space by **SET TRIMMING**

- The technique consists of applying constraints sequentially to reduce the search space

DEPARTURE FROM MATHEMATICAL PROGRAMMING

Set trimming in action



DEPARTURE FROM MATHEMATICAL PROGRAMMING

(with Marco Thiago dos Santos, André Nahes, Julia Lemos, João Domingues, Ana Levy, Aline Reyboltt) (All UERJ)

SET TRIMMING

Equipment	Original # of Candidates	Final # of Candidates	Followed by
S&T HEX	168,000	19-4000 (10 examples)	Sorting
AIR COOLER	21,600	40	Enumeration
PLATE HEX	17,000	787	Sorting
SIEVE TRAY	12,853,728	276	Sorting

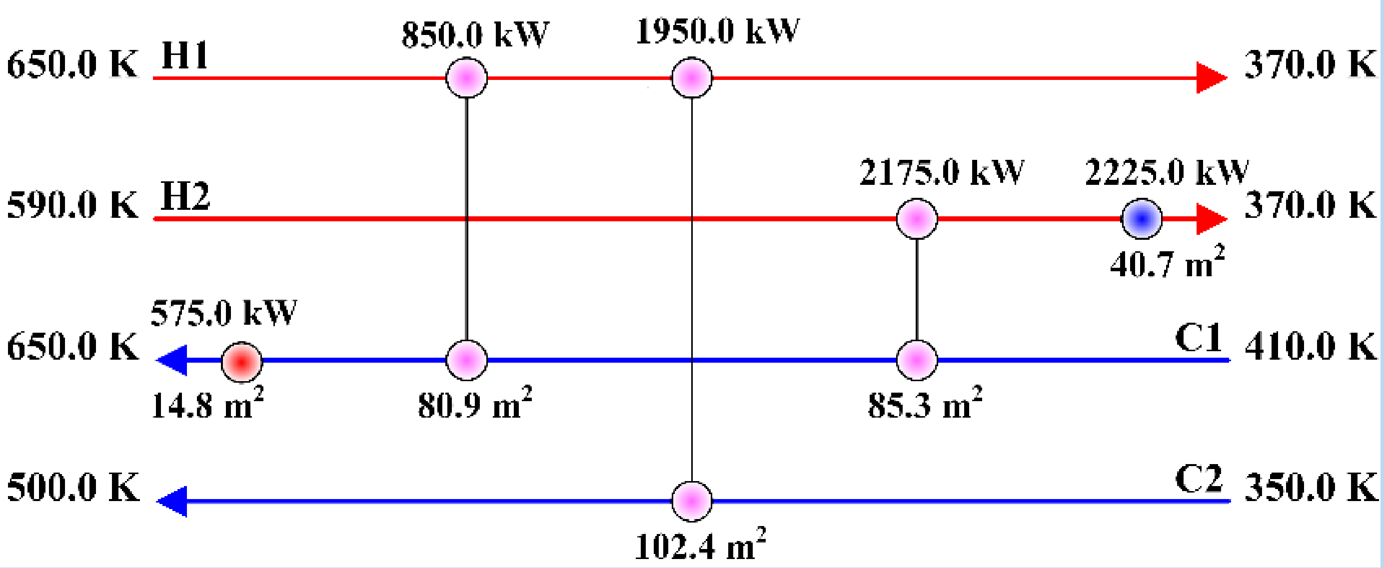
All solved in SECONDS

ADVANCES IN HEN

(with Chenglin Chang, Zuwei Liao- Zhejiang University)

Our main approach is:

- Enumeration of alternatives generated by linear models



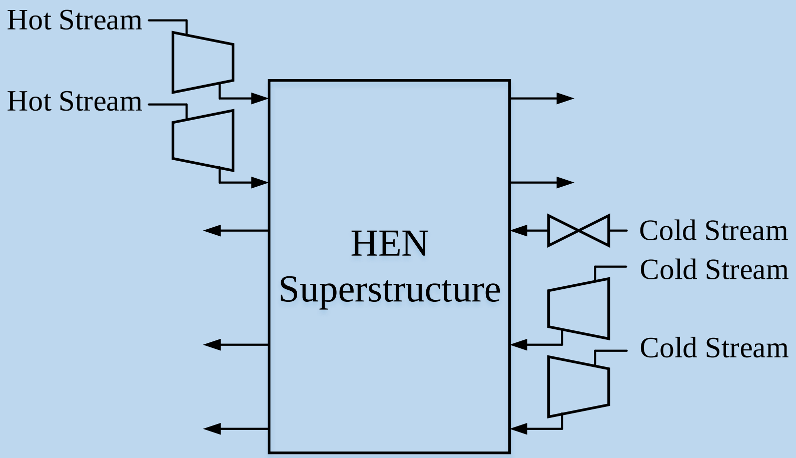
Item	Our optimal solution for Minimal HENs using different options		Best result from literature	Literature source
	Option 1	Option 4		
TAC ($/y)	155,413.1	155,413.1	154,995.0	Faria et al. (2015)
Ns	1	27	—	
Time	3.0 s	55.7 s	250.0	
TAC ($/y)	360,037.2	360,037.2	361,983.0	Escobar and Trierweiler (2013)
Ns	5	35	—	
Time	6.2 s	96.6 s	80.1	
TAC ($/y)	717,293.8	717,293.8	717,293.8	Gundersen et al. (1997)
Ns	1	5	—	
Time	4.1 s	12.6 s	Not reported	
TAC ($/y)	80,959.6	80,959.6	80,959.6	Bogataj and Kravanja (2012)
Ns	1	16	—	
Time	3.3 s	206.6 s	726.0	
TAC ($/y)	2,045,349.0	2,045,349.0	1,780,505.0	Kim et al. (2017)
Ns	3	57	—	
Time	4.8 s	198.9 s	5667.0	
TAC ($/y)	724,506.4	724,506.4	634,849.1	Escobar and Grossmann (2010)
Ns	1	101	—	
Time	1.8 s	163.6 s	3.6	
TAC ($/y)	177,261.3	177,261.3	183,029.0	Wang et al. (2016)

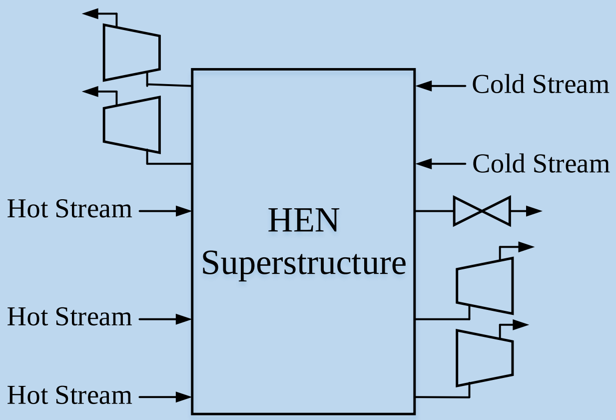
ADVANCES IN WHEN

(with Qucheng Lin, Zuwei Liao - Zhejiang University)

Our main approach is:

- Enumeration of alternatives generated by linear models. Minimal Structures



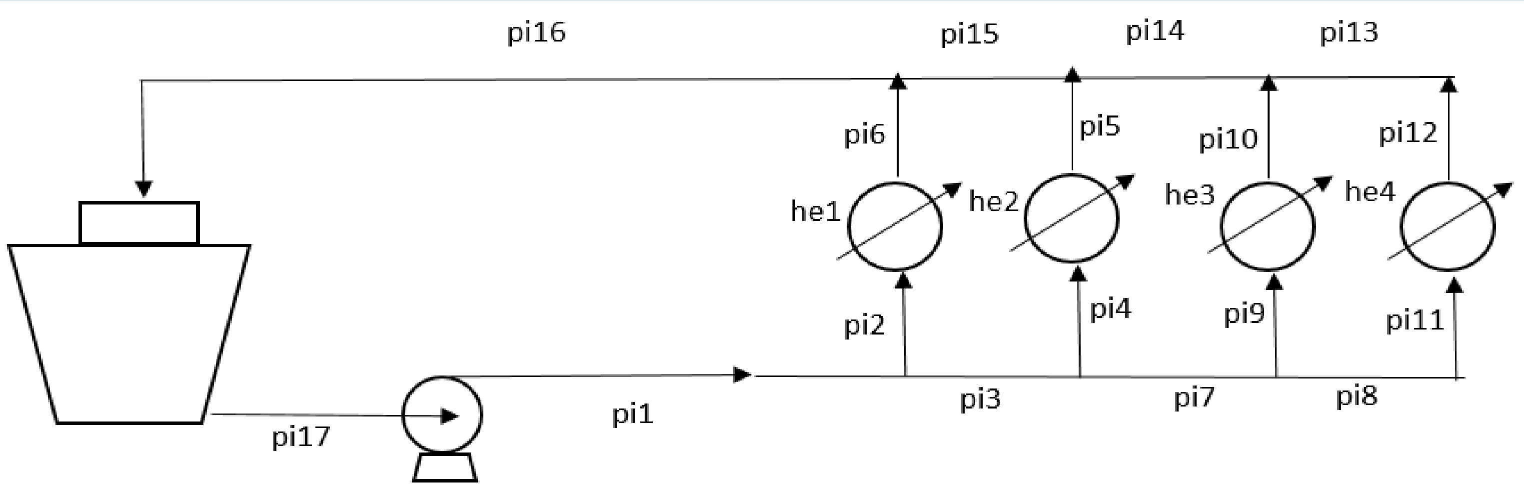


ADVANCES IN COOLING WATER SYSTEMS

(with Ana Levy-UERJ)

Our main approach is:

- Generation of linear Models aid by set trimming



USE OF DISTRIBUTED MODELS FOR EQUIPMENT DESIGN

(with Marco Thiago Dos Santos, André Nahes-UERJ)

- Classical models are based on analytical solutions obtained through simplifying assumptions (e.g. uniformity of physical properties).
- There are important engineering problems where these models are inaccurate
- Modern engineering software apply numerical methods to obtain rigorous results
- However, optimization papers usually still focus on traditional models
- Optimization tools will not be fully employed in practice if they are not based on the best available models

We substitute traditional model by rigorous models using discretization tools

PARALLEL COMPUTING & SUPERCOMPUTERS

(with Marco Thiago Dos Santos-UERJ)

Several problems for new models

- Too time consuming
- Too large. Laptops and desktops run out of memory

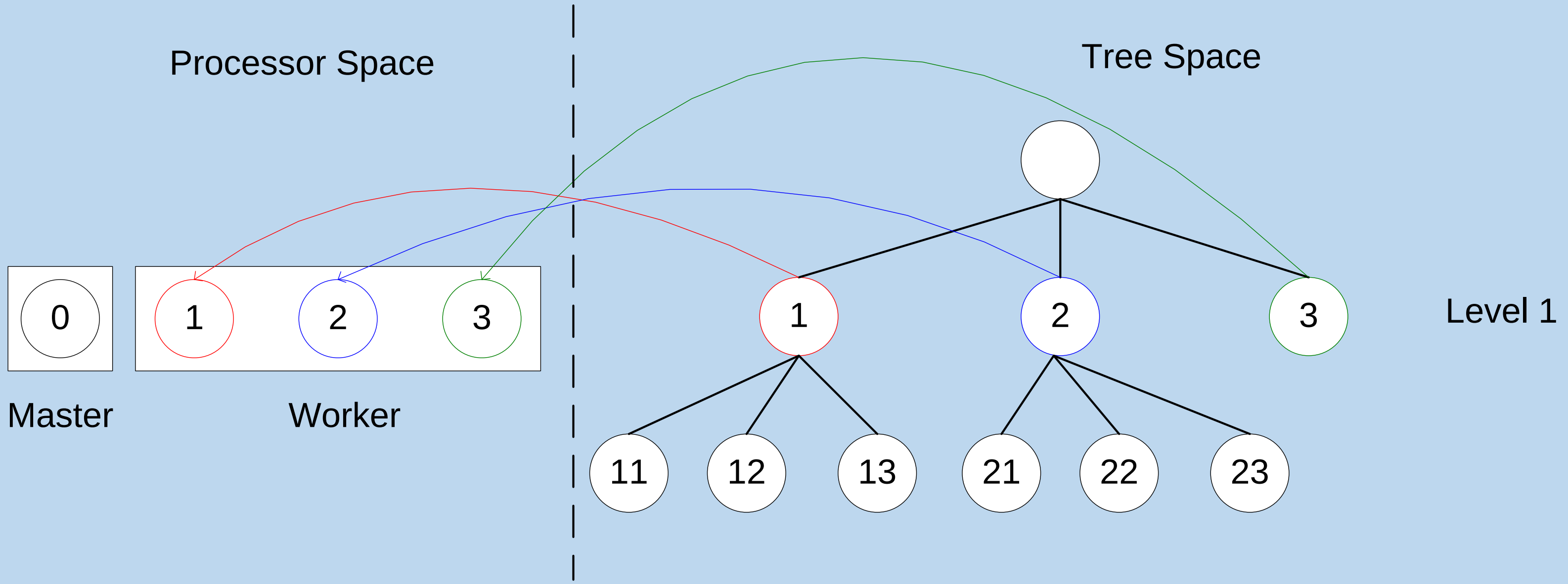
We resort to the use different processors

- By partitioning the search space
- By partitioning the search space and allow bounding and pruning

PARALLEL COMPUTING & SUPERCOMPUTERS

One processor explores one branch of the tree.

$$\left.\begin{array}{l} Min \ \sum_{\forall i} c_i \, q_i + f(x) \\ s.t. \\ \quad \sigma_k(q,x) \le 0 \qquad \forall k \in I_s \\ \quad q_i \in \{0,1\} \qquad \forall i \end{array}\right\}$$

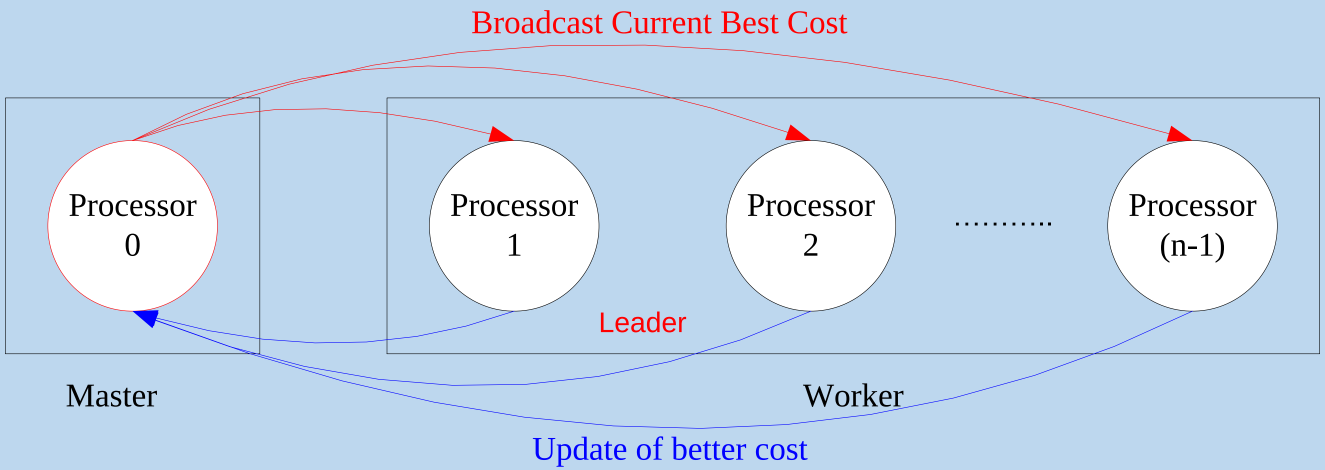


Air cooler design: 24 seconds using 25 processors

PARALLEL COMPUTING & SUPERCOMPUTERS

One processor explores one branch of the tree.
Information is broadcasted

$$\left.\begin{aligned} & Min \sum_{\forall i} c_i\, q_i + f(x) \\ & s.t. \\ & \quad \sigma_k(q,x) \le 0 \qquad \forall k \in I_s \\ & \quad q_i \in \{0,1\} \qquad \forall i \end{aligned}\right\}$$



UNCERTAINTY

(with Matheus Marques-UFRJ)

Our main approach is:

- Several correlations are based on fitting of experimental data that is dispersed.
- Deterministic models use mean value of these data
- Substitute current deterministic models (based on analytical expressions or distributed) with stochastic models

CONCLUSIONS

- Our objective is to develop new tools for equipment design and flowsheet synthesis
- We propose to get rid of heuristic procedures and use optimization methods instead
- We developed reformulation techniques that allow conversion of MINLM to MILM models
- We also developed Set Trimming techniques that many times can solve problems globally without using Mathematical Programming
- We propose to perform equipment design using distributed models
- We propose to perform synthesis of flowsheets using smart enumeration of structures
- We expect to be increasingly challenged by time and memory problems so we are working on parallel computing using supercomputers