Interactive computer based design and understanding through optimisation

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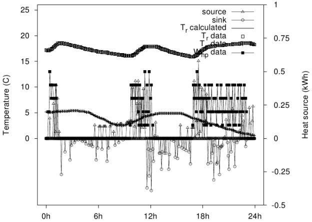
Topic

Decision support

Decision support requires analysis of possibilities

- ⇒ which must be represented by models
- ⇒ which require solving
- ⇒ to generate solutions which must be visualised.

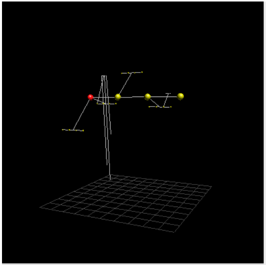


This presentation will illustrate all three aspects, from modelling through to interaction.

Process systems engineering

Models

- Can range from linear programmes (LP) through to mixed integer nonlinear dynamic algebraic programmes (MIDO).
- Represent complex systems with interactions.
- Results may be difficult to understand.



Discrete Flowsheet Viewer, design point: p78081

Applications

Chemical process design, heating systems, water distribution, etc.

Simplicity and complexity need each other.

John Maeda

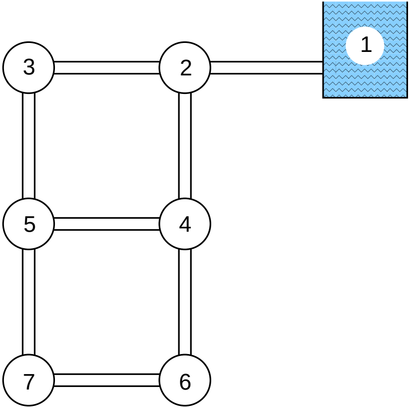
Working together

- There are three scenarios:
  1. The human does some initial work and the computer takes over.
  2. The computer solves the problem as well as it can and the user fine tunes the result.
  3. The human uses the computer iteratively to gain insight into the problem and its solutions.
- The key is to support interaction through focused computer interaction.
- An example of each is presented.

Topic

Water distribution networks

We wish to design the pipe network for water distribution for a given configuration with the aim of meeting water demand with redundancy in the network.



Example network

- 7 nodes
- 8 pipes
- 1 reservoir
- no pumps

Alperovits & Shamir (1977), Water Resource Research **13**(6):885-900

The design problem

Given

- network layout: connectivity, length (L_k), set of discrete pipe diameters, pipe cost;
- node demands, D_n; and,
- minimum head requirements, $H_n^{\min}$.

Determine

- diameter of each pipe, d_k, chosen from the set of discrete diameters;
- flow amount and direction, Q_k; and,
- head (pressure) at each node, H_n

so as to minimise total network cost.

The model

$$\min \sum_k \sum_m C_m L_k y_{km}$$

subject to:

$$\begin{aligned}
\sum_{k \in I_n} Q_k - \sum_{k \in O_n} Q_k &= D_n \\
\Delta H_k &= H_{n \in I_k} - H_{n \in O_k} \\
\Delta H_k &= w \left(\frac{Q_k}{C_{\mathrm{HW}}} \right)^{\beta} L_k \sum_m d_m^{-\gamma} y_{km} \\
H_n &\geq H_n^{\min} + E_n \\
\sum_m y_{km} &= 1
\end{aligned}$$

Indices: k, pipes/connections, n, nodes, and m, pipe diameters.

Direct optimisation

- Using state of the art optimisation solvers:

Initial Configuration	Solution (10^3) CONOPT2	CONOPT3	MINOS	MINOS5
None	659	655	444	Fails
All flows $= 100$	441	441	452	452

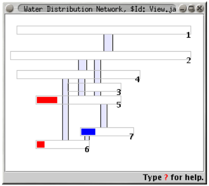
- Initialisation affects success of the NLP solvers.

$\Rightarrow$ Let human initialise the problem using a graphical representation.

Discrete optimization

Use of visualization requires mapping from continuous to discrete space.

- Mapping converts MINLP to discrete programming model …
- … but equality constraints cannot be satisfied in discrete space.
- So we use interval analysis to identify solutions which are close to feasible in discrete space.



The discrete model is solved either by the engineer through interaction or using an embedded stochastic optimisation procedure.

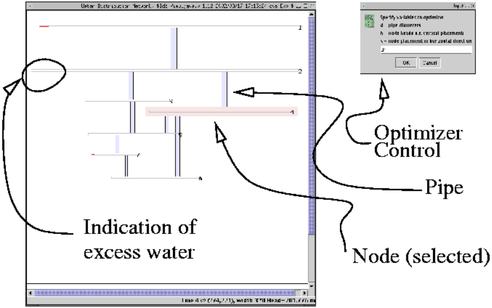
Interval arithmetic

Changes to model given that node heads are now intervals:

$$
\begin{aligned}
\boxed{\Delta H_k} &= \boxed{H_{n \in I_k}} - \boxed{H_{n \in O_k}} \\
\boxed{Q_k} &= \left(\frac{\boxed{\Delta H_k}}{w \frac{L_k}{C^\beta d_k^\gamma}} \right)^{\frac{1}{\beta}} \\
0 &\in \sum_{k \in I_n} \boxed{Q_k} - \sum_{k \in O_n} \boxed{Q_k} - D_n
\end{aligned}
$$

where $\boxed{}$ indicates an interval value.

Demonstration



www

ESF & Papageorgiou (2007), Optimization and Its Applications, Springer, **4**:311-332.

Improved results

Initial Configuration	Solution (10^3) conopt2	conopt3	minos	minos5
None	659	655	444	Fails
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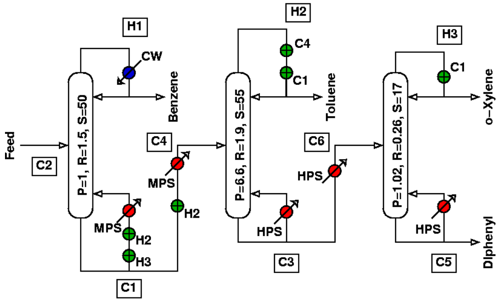
Improved results

Initial Configuration	Solution (10^3) conopt2	conopt3	minos	minos5
None	659	655	444	Fails
All flows = 100	441	441	452	452
Human	419	419	423	419

- Behaviour of NLP solvers is more consistent.
- Solutions obtained are better in all cases.
- The best known solution is found in 3 of the cases.

Topic

Heat integrated process design



Goals

- Identify process steps and interconnections.
- Design and cost individual processing units and exchangers.
- Understand possible solutions and their constraints.

Methodology

Use interaction to fine-tune computer generated designs.

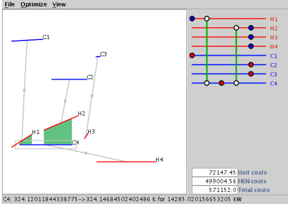
To simplify complications is the first essential of success.

George Earle Buckle

Visual representation

Hot and cold streams

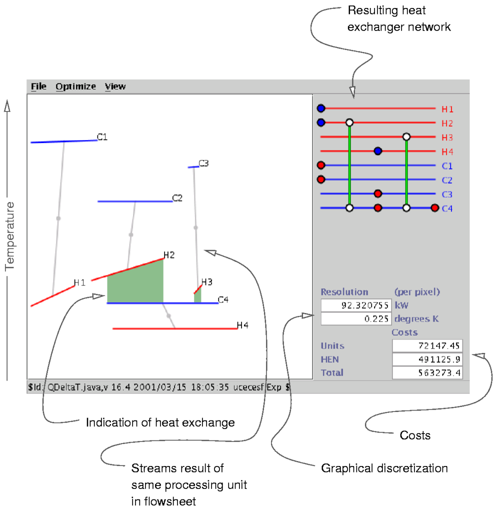
- Colour indication of stream type.
- x-axis for position independent duties.
- y-axis for temperature.
- Overlapping hot over cold streams indicates heat integration.



Methdology

The tail wagging dog approach: user interaction with streams modifies the underlying process to achieve desired integration.

Interactive tool

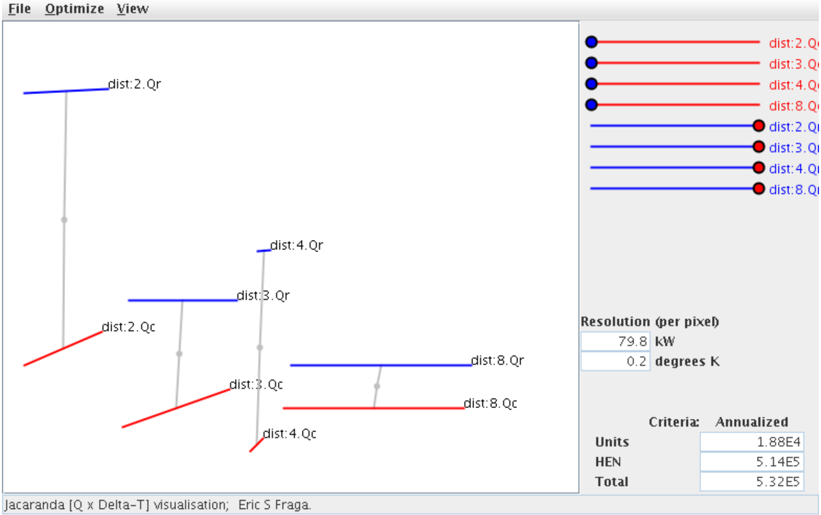


- Immediate feedback encourages exploration and allows for insight.
- Caveat: the design space is complex and large so the best solutions are not always immediately obvious.
- Automation of search is possible.

www

ESF, Patel & Rowe (2001). ChERD **79**(7):765–776

Demonstration of interaction



Automated search

Representation

A graphical view of process heat requirements defines left and right end-points for each hot and cold stream in the process:

$$\{(x_{a,i}, y_{a,i})\}$$

$$\{(x_{b,i}, y_{b,i})\}$$

$i = 1, \ldots, n_s$ and $x, y \in \mathbb{Z}^+$, suitable for manipulation by evolutionary algorithms.

Evaluation

1. Define list of intervals

$$I \leftarrow \bigcup_{1}^{n_s} \{\{x_{a,i}\} \cup \{x_{b,i}\}\}$$

2. For each interval $[I_j, I_{j+1}]$:
   1. Enumerate active streams.
   2. Sort streams.
   3. Identify matches.
   4. Quantify utility requirements
3. Coalesce adjacent matches.
4. Design exchangers.
5. Generate objective function values.

Suitable for use with an integer optimisation procedure.

Demonstration

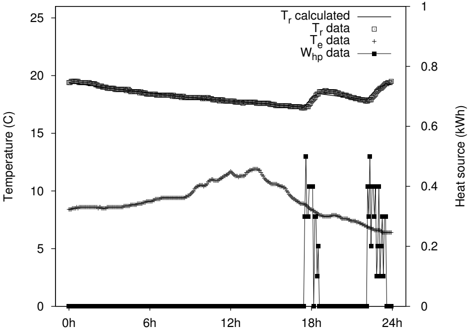
www

Topic

Heating for dwellings

The dwelling

- An air source heat pump is used to provide heating.
- We need to understand the behaviour of the dwelling.
- This requires a model of the heat balances.
- Data are available at 5 minute intervals.



Zhang, Papageorgiou, ESF (2012), Proc ESCAPE 22.

Model fitting

Fitting data to a model consists of identifying the values of the free parameters which minimise some estimate of the error in the fit.

Optimisation problem definition

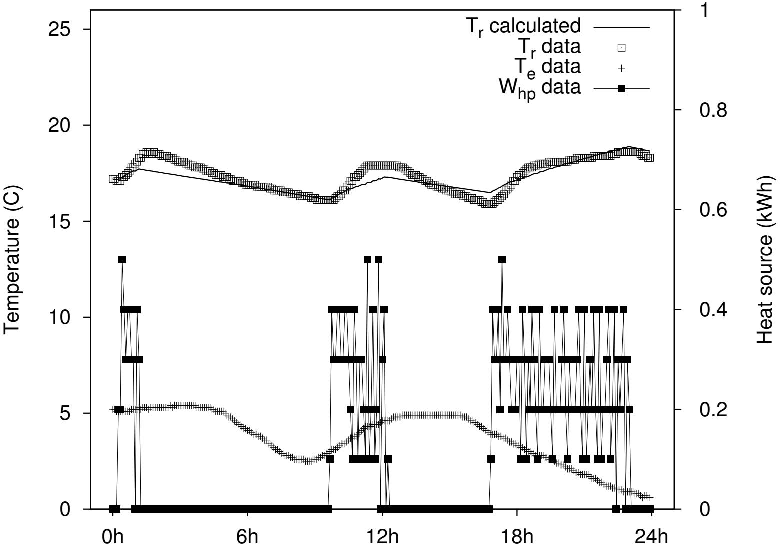
$$\min_{C,L} z = \| T_r - \hat{T}_r \| \tag{1}$$

subject to

$$C \frac{\mathrm{d}}{\mathrm{d}t} T_r(t) = W_{\mathrm{hp}}(t) - L \Delta T(t) \qquad t \in [t_1, t_n]$$

This is a dynamic nonlinear programming (DNLP) problem for the minimisation of z by manipulation of C and L subject to the dynamic model for the behaviour of the room temperature.

Example solution: 30 November



Question

Why is the fit not good?

More questions

Premise

The model is not a good representation of what is happening.

Questions

- Is a linear driving force for heat transfer appropriate?
- Are dynamics properly represented?
- Are there missing sources and sinks of heat?

We can explore each of these questions in turn through further modelling and by applying optimisation techniques.

Eventually: improved model

Extend the model

$$C\frac{\mathrm{d}}{\mathrm{d}t}T_r(t) = W_{\mathrm{hp}}(t-\lambda_2) - \Delta T(t-\lambda_1)\cdot(\alpha+\gamma\Delta T^2) + W_{\mathrm{so}}(t) - W_{\mathrm{si}}(t)$$

with

1. time delays,
2. a nonlinear driving force,
3. adding extra terms for unknown sources and sinks,

and new optimisation variables α, γ, λ_1, λ_2, $W_{\mathrm{so}}(t)$, $W_{\mathrm{si}}(t)$.

Penalty based objective function

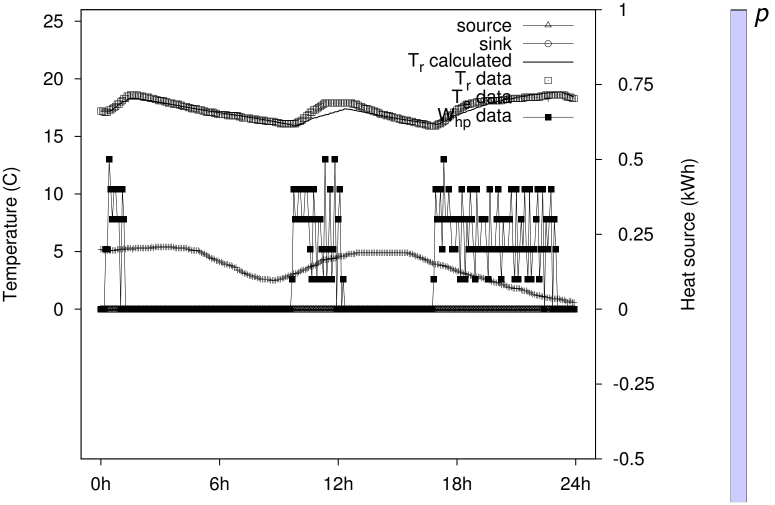
$$\min z = \| T_r - \hat{T}_r \| + \boxed{p \left(\| W_{\mathrm{so}} \| + \| W_{\mathrm{si}} \| \right)} \quad p \geq 0$$

s.t.

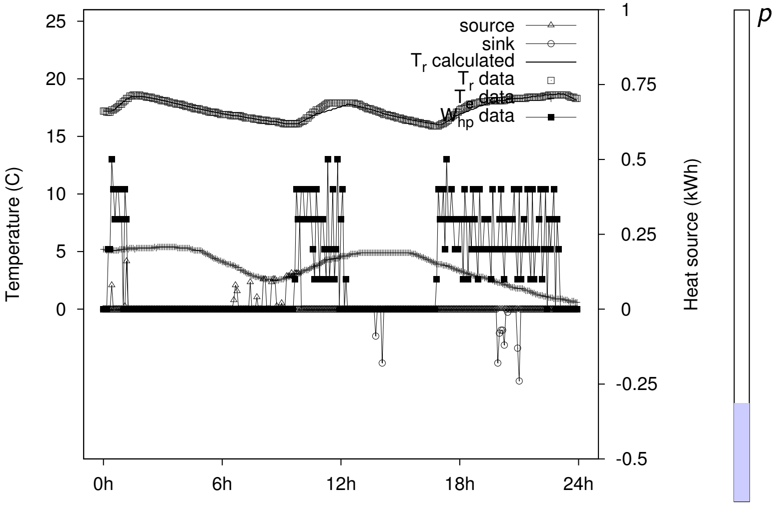
$$\begin{aligned} C \frac{\mathrm{d}}{\mathrm{d}t} T_r(t) = {} & W_{\mathrm{hp}}(t - \lambda_2) \\ & - \left(\alpha + \gamma \Delta T^2 \right) \Delta T (t - \lambda_1) \qquad t \in [t_1, t_n] \\ & + W_{\mathrm{so}}(t) - W_{\mathrm{si}}(t) \end{aligned}$$

The penalty factor, p, controls the relative importance of the slack variables.

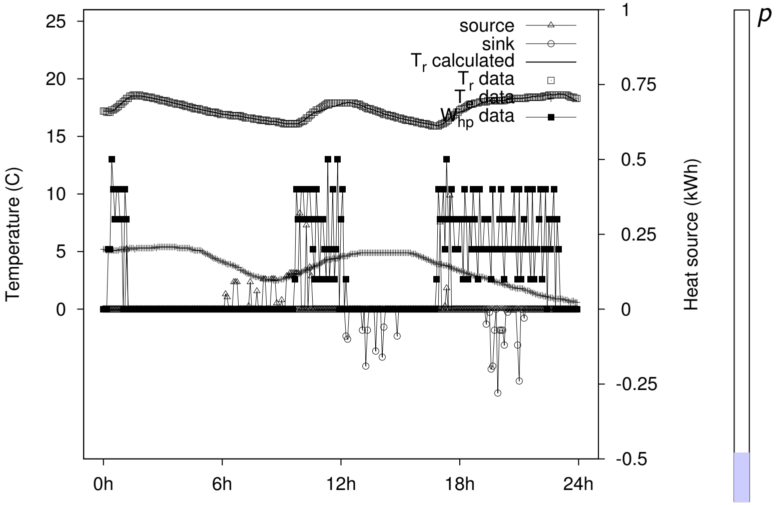
Numerical experiments



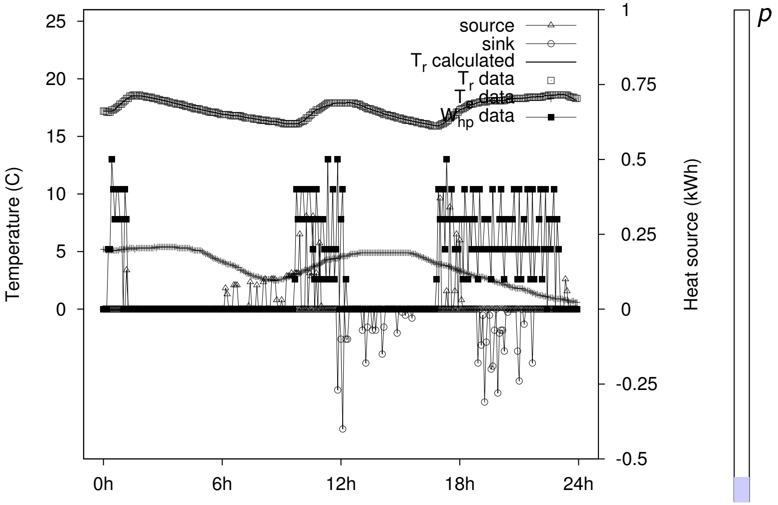
Numerical experiments



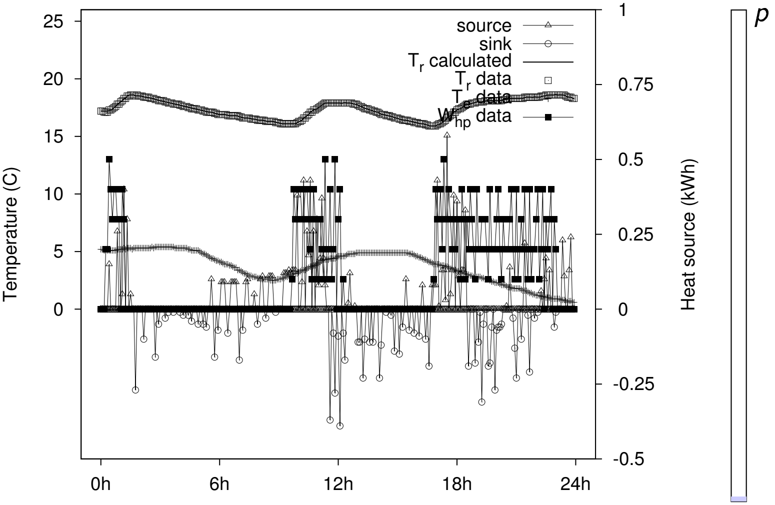
Numerical experiments



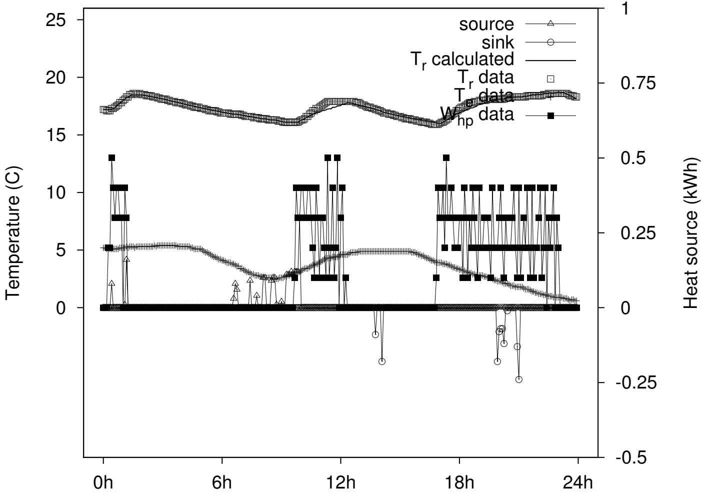
Numerical experiments



Numerical experiments



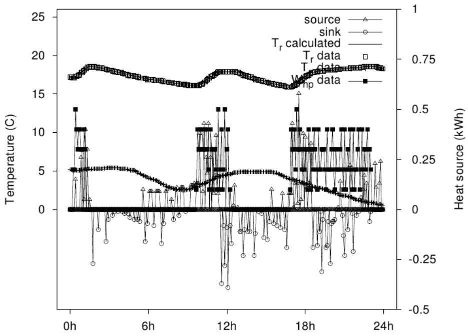
Updated solution: 30 November



Topic

Summary

- Modelling is an iterative procedure:
  - generate results
  - analyse them
  - revise model
  - repeat
- Optimisation is not just about finding the best solution but can provide insight.
- Insight may lead to better decisions.



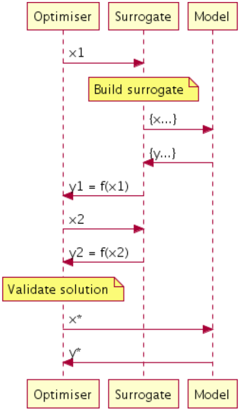
Current projects

Methodological

- Surrogate modelling.
- Handling fuzzy metrics.

Applications

- Carbon capture for power plants.
- Heat integrated biofuel process design.
- Systems integration for renewable energy.
- CO_2 as a raw material feedstock.
- Water splitting for Hydrogen production.
- Water processing for coal seam gas.



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