Optimal Control in Chemical Engineering

From Roger W.H. Sargent to the Present and Future

Vassilis S. Vassiliadis

Process Systems Engineering (PSE) Research Group
Department of Chemical Engineering and Biotechnology
University of Cambridge

Roger W.H. Sargent Memorial

Imperial College London

4 April 2019

About this talk...!

"You can talk about Optimal Control, but ...:"

- *"Bear in mind it is for a general audience"*
  ($\Longrightarrow$no maths during entire talk $\equiv$ "path constraint"!)

- *"You have 20 minutes only to complete it"*
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$\longrightarrow$ reduce material, "*SpeedUp*" presentation!

Outline

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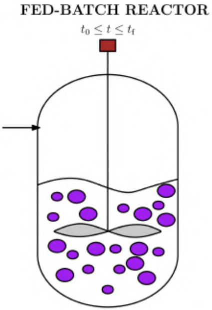
Definition of OCP



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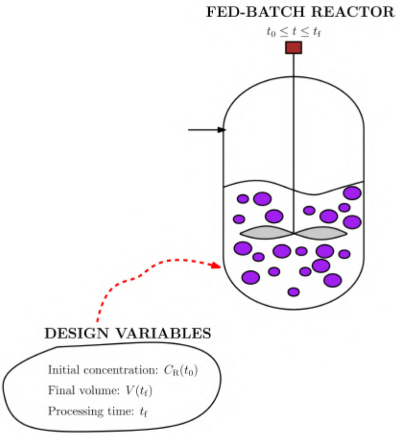

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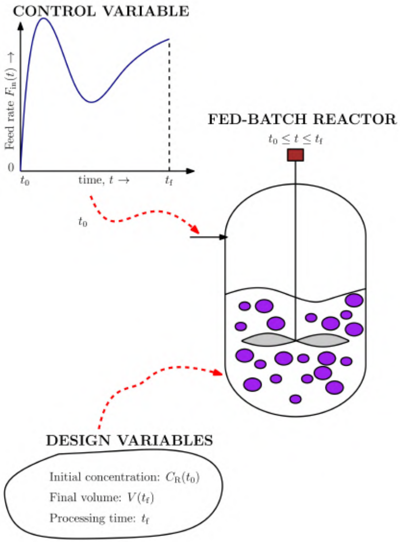

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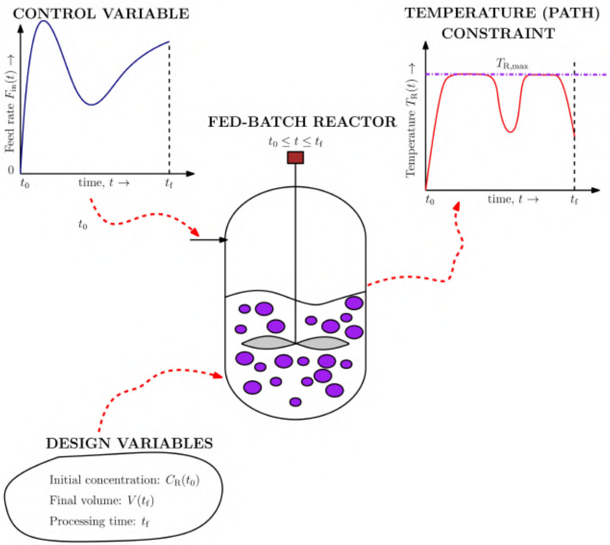

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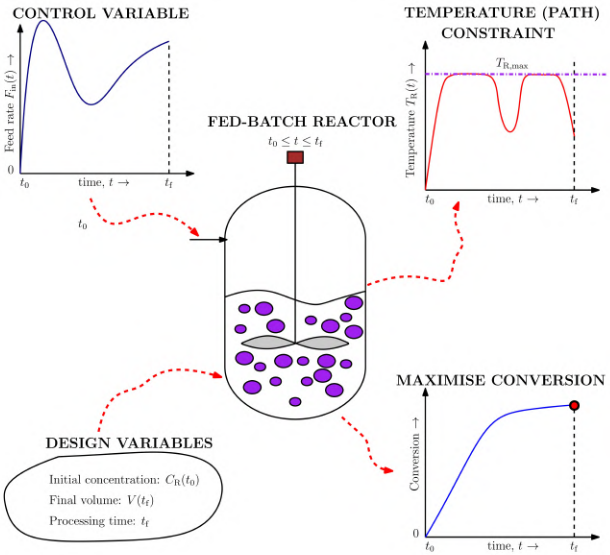
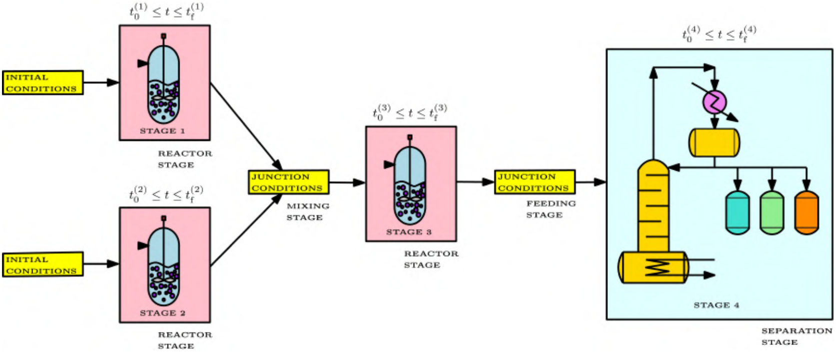


Multistage systems



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Origins of optimal control: calculus of variations

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  - Bernoulli (brachystochrone problem)
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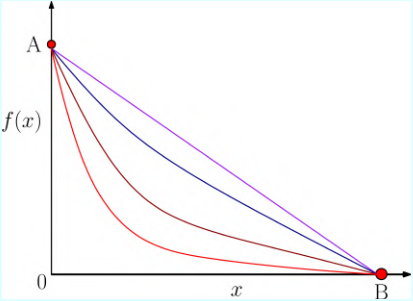

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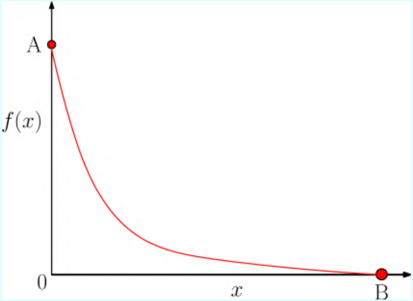

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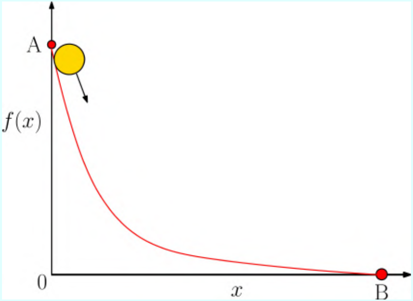

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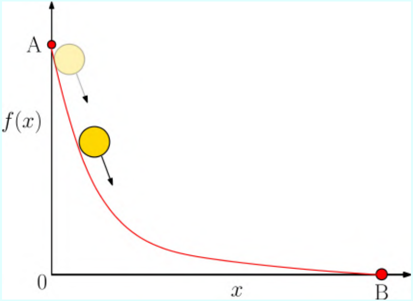

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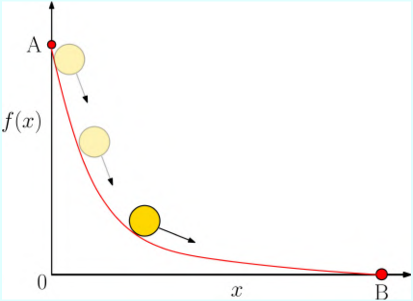

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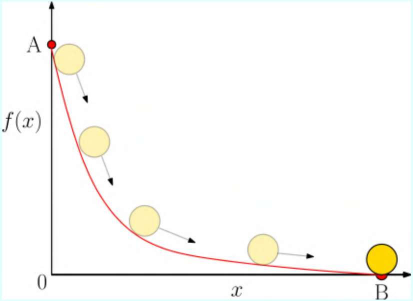

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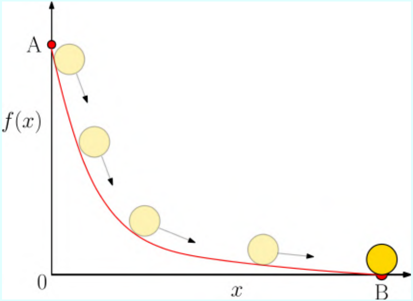

- Analytical approach (calculus of variations)
  - Euler & Lagrange (problem formulation)
  - Legendre, Jacobi, Weierstrass (necessary conditions)
  - Carathéodory (existence of solutions)
  - Pontryagin (maximum principle)

Outline

Foundation of Process Systems Engineering (PSE)

CEP
CHEMICAL ENGINEERING PROGRESS

INTEGRATED DESIGN AND OPTIMIZATION OF PROCESSES

R. W. H. Sargent

Imperial College of Science and Technology,
University of London, London, England

Vol. 63, No. 9 SEPTEMBER 1967 Pages 71-78

Foundation of Process Systems Engineering (PSE)

R. W. H. Sargent received his B.Sc. and Ph.D. in chemical engineering from Imperial College. From October 1951 to May 1958 he was with Société L'Air Liquide, Paris, in the Département Etudes Liquéfaction. He was in charge of Process Design Section at the time of leaving. He is currently Courtaulds Professor of Chemical Engineering, Imperial College. Sargent is member of Council of The Institution of Chemical Engineers and chairman of its Publications Committee.

VOL

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Although we are in sight of a truly integrated approach to the design of complete processes, a great deal of work remains to be done. With the need for more sophisticated analysis of larger complexes, it is more than ever necessary to join hands with those working in the fields of control engineering, operational research, numerical analysis, and computer science.

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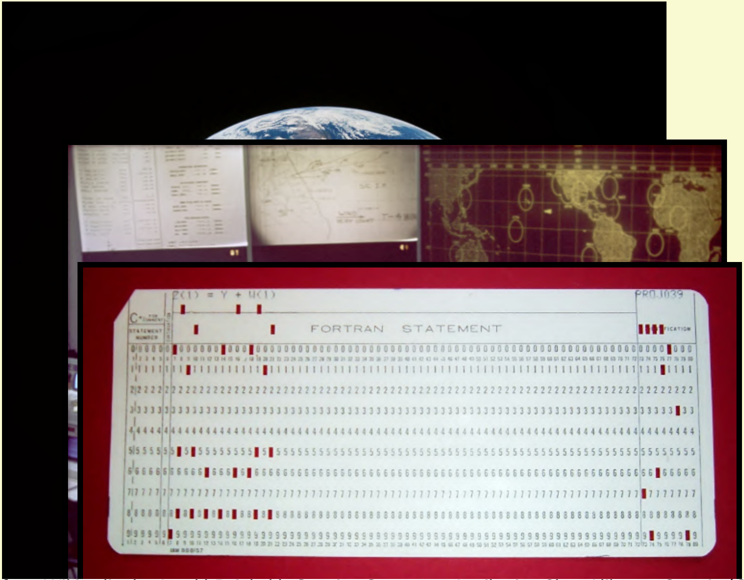

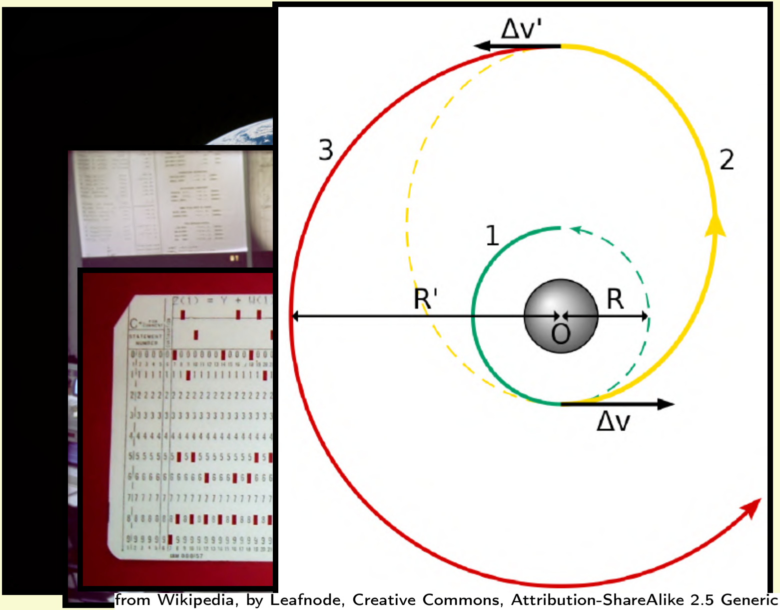
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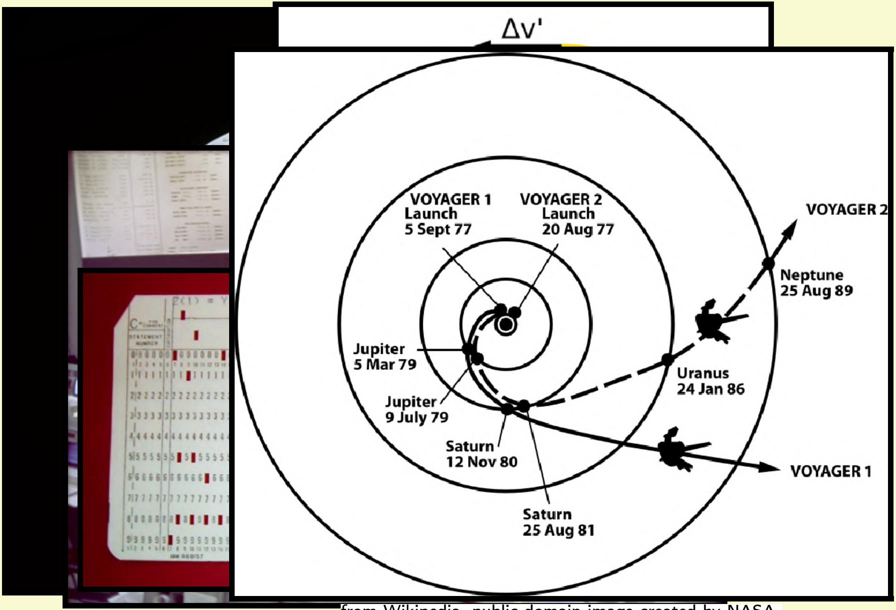

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PREDICTION AND OPTIMISATION

OF THE DYNAMIC PERFORMANCE OF A DISTILLATION COLUMN

A thesis submitted for

the Degree of Doctor of Philosophy

in the Faculty of Engineering of the University of London

by

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July 1967.

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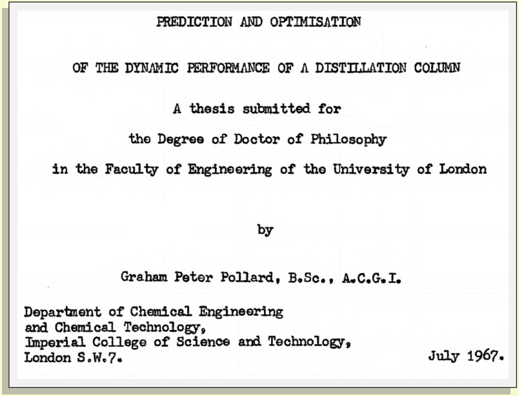

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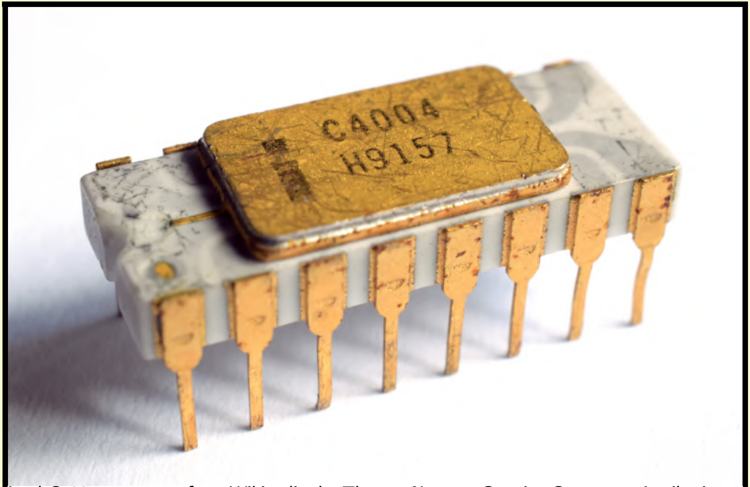

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Apple I computer, from Wikipedia, by Ed Uthman, Creative Commons, Attribution-ShareAlike 2.0 Generic (CC BY-SA 2.0), https://creativecommons.org/licenses/by-sa/2.0/deed.en

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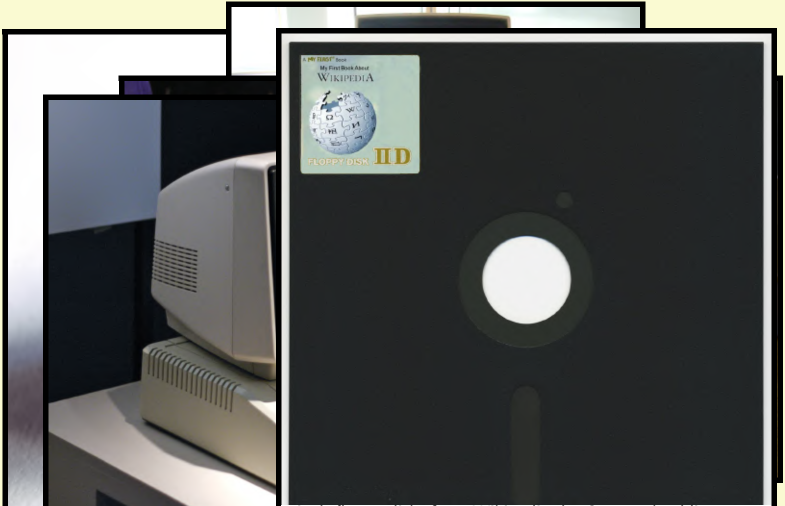

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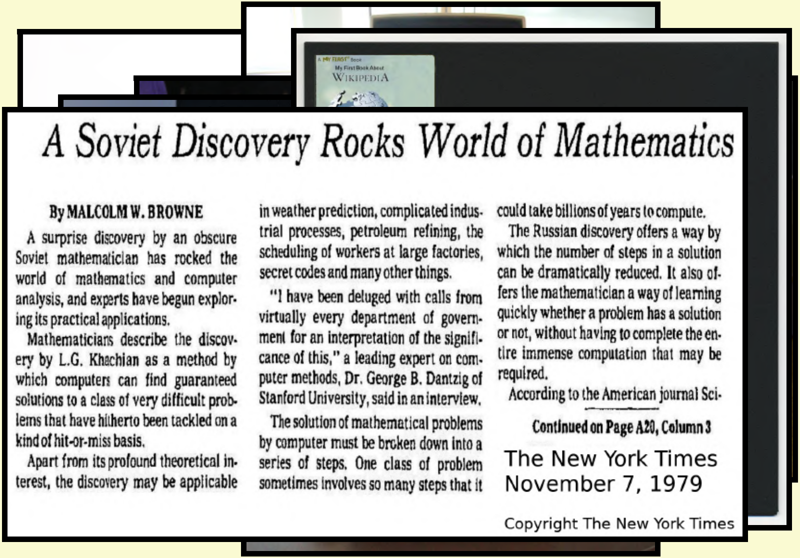


A Soviet Discovery Rocks World of Mathematics

By MALCOLM W. BROWNE

A surprise discovery by an obscure Soviet mathematician has rocked the world of mathematics and computer analysis, and experts have begun exploring its practical applications.

Mathematicians describe the discovery by L.G. Khachian as a method by which computers can find guaranteed solutions to a class of very difficult problems that have hitherto been tackled on a kind of hit-or-miss basis.

Apart from its profound theoretical interest, the discovery may be applicable in weather prediction, complicated industrial processes, petroleum refining, the scheduling of workers at large factories, secret codes and many other things.

"I have been deluged with calls from virtually every department of government for an interpretation of the significance of this," a leading expert on computer methods, Dr. George B. Dantzig of Stanford University, said in an interview.

The solution of mathematical problems by computer must be broken down into a series of steps. One class of problem sometimes involves so many steps that it could take billions of years to compute.

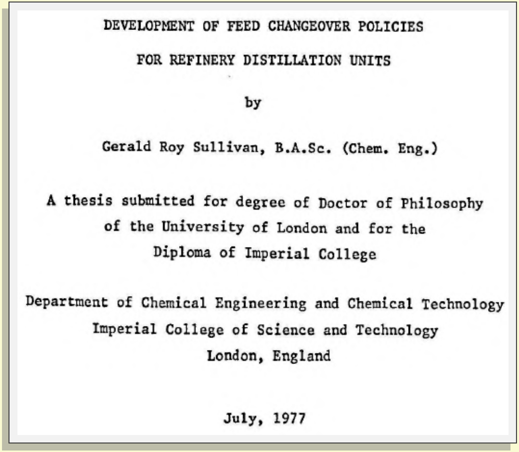
The Russian discovery offers a way by which the number of steps in a solution can be dramatically reduced. It also offers the mathematician a way of learning quickly whether a problem has a solution or not, without having to complete the entire immense computation that may be required.

According to the American journal Sci-

Continued on Page A20, Column 3

The New York Times
November 7, 1979

Line at a gas station in Maryland, June 15, 1979, from Wikipedia, from the U.S. News & World Report collection at the Library of Congress, public domain



DEVELOPMENT OF FEED CHANGEOVER POLICIES

FOR REFINERY DISTILLATION UNITS

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July, 1977

Aim:

Changeover policies for refinery distillation, full scale OCP package development.

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- Optimisation: variable metric projection method,
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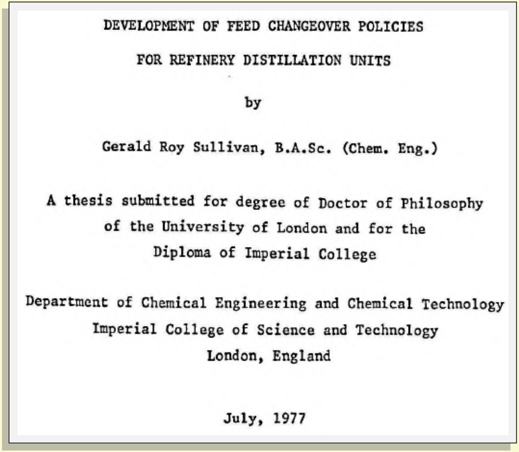
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IBM PC 5150, August 1981, from Wikipedia, by "Boffy b", Creative Commons, Attribution-ShareAlike 1.0 Generic (CC BY-SA 1.0), https://creativecommons.org/licenses/by-sa/1.0/deed.en

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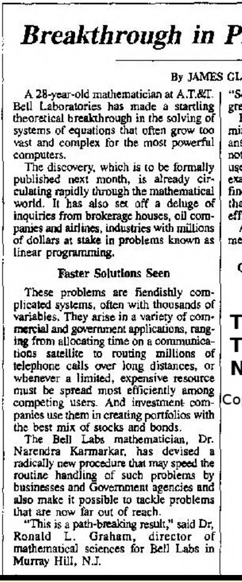

Breakthrough in Problem Solving

By JAMES GLEICK

A 28-year-old mathematician at A.T.&T. Bell Laboratories has made a startling theoretical breakthrough in the solving of systems of equations that often grow too vast and complex for the most powerful computers.

The discovery, which is to be formally published next month, is already circulating rapidly through the mathematical world. It has also set off a deluge of inquiries from brokerage houses, oil companies and airlines, industries with millions of dollars at stake in problems known as linear programming.

Faster Solutions Seen

These problems are fiendishly complicated systems, often with thousands of variables. They arise in a variety of commercial and government applications, ranging from allocating time on a communications satellite to routing millions of telephone calls over long distances, or whenever a limited, expensive resource must be spread most efficiently among competing users. And investment companies use them in creating portfolios with the best mix of stocks and bonds.

The Bell Labs mathematician, Dr. Narendra Karmarkar, has devised a radically new procedure that may speed the routine handling of such problems by businesses and Government agencies and also make it possible to tackle problems that are now far out of reach.

"This is a path-breaking result," said Dr. Ronald L. Graham, director of mathematical sciences for Bell Labs in Murray Hill, N.J.

"Science has its moments of great progress, and this may well be one of them."

Because problems in linear programming can have billions or more possible answers, even high-speed computers cannot check every one. So computers must use a special procedure, an algorithm, to examine as few answers as possible before finding the best one — typically the one that minimizes cost or maximizes efficiency.

A procedure devised in 1947, the simplex method, is now used for such problems.

Continued on Page A19, Column 1

THE NEW YORK TIMES, November 19, 1984

AT&T Markets Problem Solver, Based On Math Whiz's Find, for $8.9 Million

By ROGER LOWENSTEIN
Staff Reporter of THE WALL STREET JOURNAL

NEW YORK—American Telephone & Telegraph Co. has called its math whiz, Narendra Karmarkar, a latter-day Isaac Newton. Now, it will see if he can make the firm some money.

Four years after AT&T announced an "astonishing" discovery by the Indian-born Mr. Karmarkar, it is marketing an $8.9 million problem solver based on his invention.

Dubbed Korbx, the computer-based system is designed to solve major operational problems of both business and government. AT&T predicts "substantial" sales for the product, but outsiders say the price is high and point out that its commercial viability is unproven.

"At $9 million a system, you're going to have a small number of users," says Thomas Magnanti, an operations-research specialist at Massachusetts Institute of Technology. "But for very large-scale problems, it might make the difference."

Korbx uses a unique algorithm, or step-by-step procedure, invented by Mr. Karmarkar, a 32-year old, an AT&T Bell Laboratories mathematician.

"It's designed to solve extremely difficult or previously unsolvable resource-allocation problems—which can involve hundreds of thousands of variables—such as personnel planning, vendor selection, and equipment scheduling," says Aristides Fronistas, president of an AT&T division created to market Korbx.

Potential customers might include an airline trying to determine how to route many planes between numerous cities and an oil company figuring how to feed different grades of crude oil into various refineries and have the best blend of refined products emerge.

AT&T says that fewer than 10 companies, which it won't name, are already using Korbx. It adds that, because of the price, it is targeting only very large companies—mostly in the Fortune 100.

Korbx "won't have a significant bottom-line impact initially" for AT&T, though it might in the long term, says Charles Nichols, an analyst with Bear, Stearns & Co. "They will have to expose it to users and demonstrate" it uses.

AMR Corp.'s American Airlines says it's considering buying AT&T's system. Like other airlines, the Fort Worth, Texas, carrier has the complex task of scheduling pilots, crews and flight attendants on thousands of flights every month.

Thomas M.Cook, head of operations research at American, says, "Every airline has programs that do this. The question is: Can AT&T do it better and faster? The jury is still out."

The U.S. Air Force says it is considering using the system at the Scott Air Force Base in Illinois.

One reason for the uncertainty is that AT&T has, for reasons of commercial secrecy, deliberately kept the specifics of Mr. Karmarkar's algorithm under wraps.

"I don't know the details of their system," says Eugene Bryan, president of Decision Dynamics Inc., a Portland, Ore., consulting firm that specializes in linear programming, a mathematical technique that employs a series of equations using many variables to find the most efficient way of allocating resources.

Mr. Bryan says, though, that if the Karmarkar system works, it would be extremely useful. "For every dollar you spend on optimization," he says, "you usually get them back many-fold."

AT&T has used the system in-house to help design equipment and routes on its Pacific Basin system, which involves 22 countries. It's also being used to plan AT&T's evolving domestic network, a problem involving some 800,000 variables.

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Mathematical Programming 36 (1986) 183–209
North-Holland

ON PROJECTED NEWTON BARRIER METHODS FOR LINEAR PROGRAMMING AND AN EQUIVALENCE TO KARMARKAR'S PROJECTIVE METHOD

Philip E. GILL, Walter MURRAY, Michael A. SAUNDERS

Department of Operations Research, Stanford University, Stanford, CA 94305, USA

J.A. TOMLIN

Ketron Incorporated, Mountain View, California 94040, USA

Margaret H. WRIGHT

Department of Operations Research, Stanford University, Stanford, CA 94305, USA

Received 12 October 1985
Revised manuscript received 20 June 1986

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The Interior Point Revolution Begins!!!

OPTIMAL CONTROL OF PROCESSES DESCRIBED

BY SYSTEMS OF

DIFFERENTIAL-ALGEBRAIC EQUATIONS

by

Ken R. Morison

October 1984

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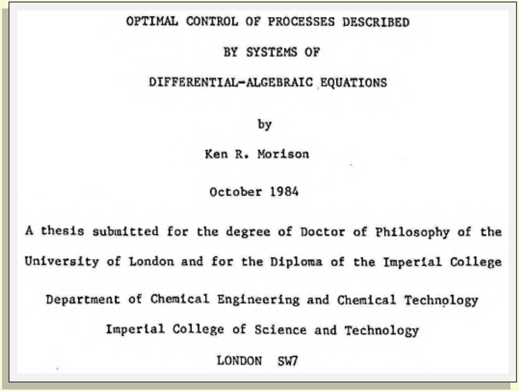
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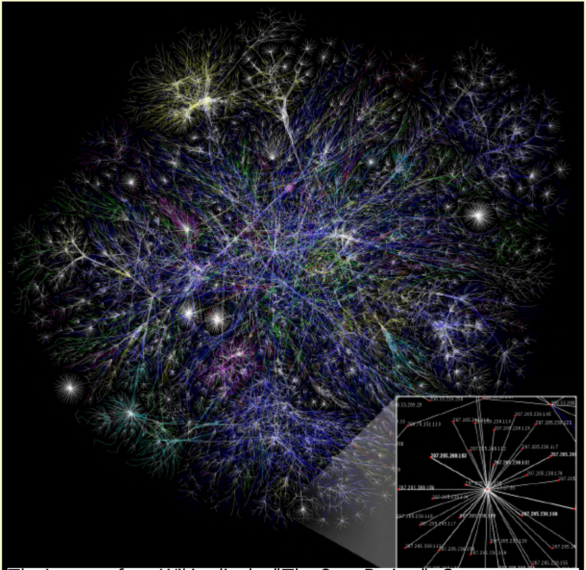

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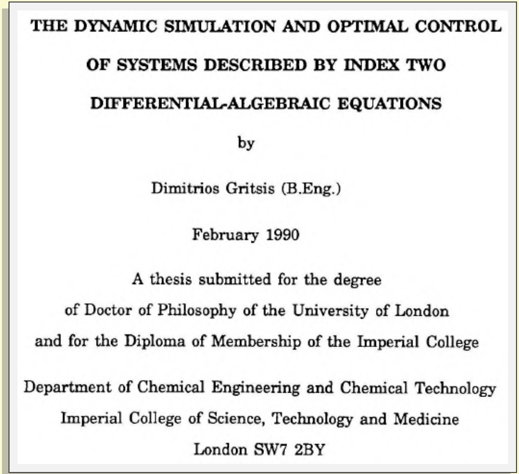


THE DYNAMIC SIMULATION AND OPTIMAL CONTROL

OF SYSTEMS DESCRIBED BY INDEX TWO

DIFFERENTIAL-ALGEBRAIC EQUATIONS

by

Dimitrios Gritsis (B.Eng.)

February 1990

A thesis submitted for the degree

of Doctor of Philosophy of the University of London

and for the Diploma of Membership of the Imperial College

Department of Chemical Engineering and Chemical Technology

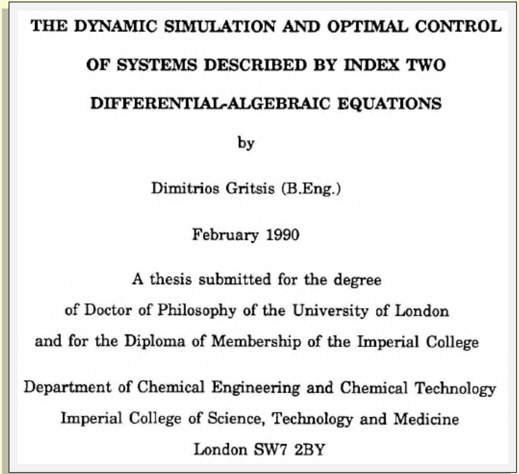
Imperial College of Science, Technology and Medicine

London SW7 2BY

Aim:

The dynamic simulation and optimal control of systems described by index-2 DAEs.

- DAE systems of index-2,
- Gradients: adjoint equations.



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Computational Solution of Dynamic Optimization Problems with General Differential-Algebraic Constraints

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General OCPs with general constraints.

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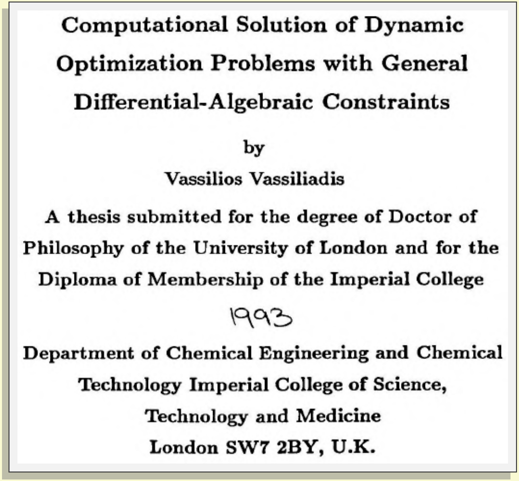
- Multistage OCP systems,
- Gradients: sensitivity equations,
- Treatment of inequality path constraints,
- `DAEOPT`: a generic large-scale OCP solver.



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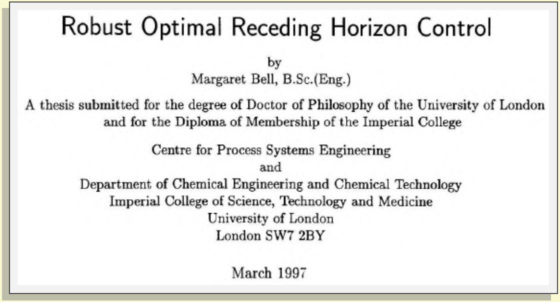
Robust Optimal Receding Horizon Control

by
Margaret Bell, B.Sc.(Eng.)

A thesis submitted for the degree of Doctor of Philosophy of the University of London
and for the Diploma of Membership of the Imperial College

Centre for Process Systems Engineering
and
Department of Chemical Engineering and Chemical Technology
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London SW7 2BY

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Aim:

Receding horizon control.

- Interior point formulation for path constraints,
- Robustness considerations.

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Journal of Computational and Applied Mathematics 124 (2000) 361–371

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Optimal control

R.W.H. Sargent *

Centre for Process Systems Engineering, Imperial College, Prince Consort Road, London SW7 2BY, UK

Received 20 August 1999; received in revised form 25 November 1999

- Historical review,
- Calculus of variations,
- Optimal control theory,
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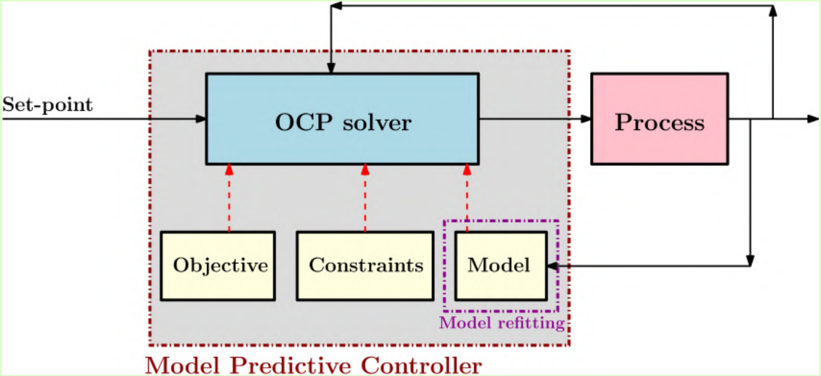
Outline

1/5: Nonlinear Model Predictive Control (NMPC)



A commercially available methodology:

- gPROMS dynamic simulator by Process Systems Enterprise LTD.,
- feasible path approach for mixed-integer dynamic optimisation problems.

3/5: MIOCP without B&B!

- Contribution by Sebastian Sager[1]:
  - Reformulation of MIOCP in relaxed and convexified form,
    - ODE/DAE models affine in the control,
  - Bang-bang solutions $\rightarrow$ 0-1 behaviour of binary controls.
- Extended to multistage systems by PSE group at Cambridge University.

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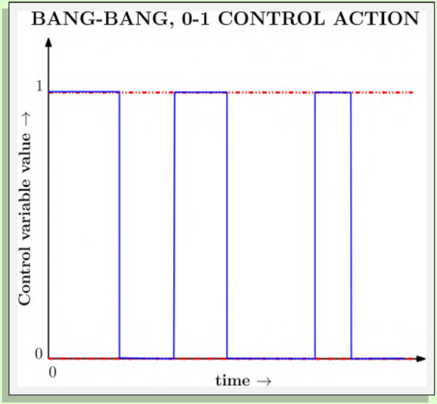

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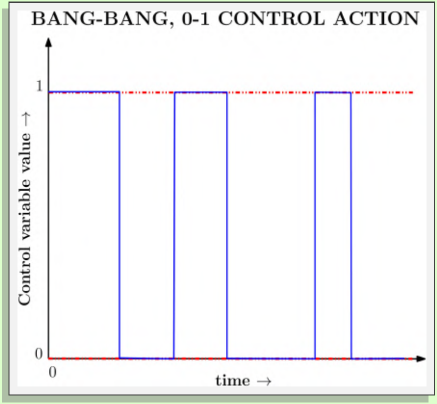

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Application: maintenance scheduling of HENs subject to fouling[1]

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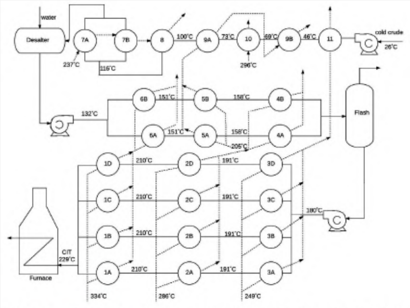

Fig. 3. 25 unit HEN case. Solid lines, cold (crude) streams; dashed lines, hot streams; CIT, crude inlet temperature to furnace. Temperature values are given for initial, clean condition. Adapted from Smaïli et al., 2002a.

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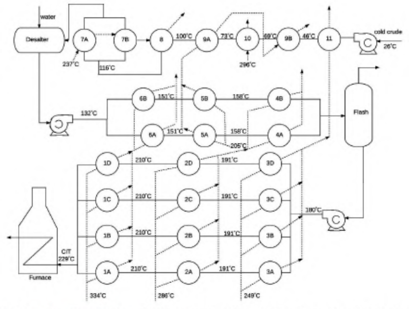

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Table 16
Cleaning schedule for the 25 unit HEN case (linear fouling, cleaning cost = £5k).

HEX	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	No. of cleaning actions +	No. of cleaning actions ○
1A												○					+								+	○											2	2
1B													+	○													⊖										2	2
1C												+	○												○	+											2	2
1D											○					+								○				+									2	2
2A										+					○								+				○										2	2
2B														+		○										⊖											2	2
2C														○		+								○			+										2	2
2D												+	○												⊖												2	2
3A																		+																			1	0
3B															+																						1	0
3C																	+	○																			1	1
3D																	○		+																		1	1
4A												○			+													⊖									2	2
4B									+	○													○	+													2	2
5A																	+	○																			1	1
5B																	○	+																			1	1
6A										○				+									○	+													2	2
6B															+			○					+														2	1
7A															+		○																				1	1
7B																		+				○															1	1
8																			⊖																		1	1
9A																				⊖																	1	1
9B												○	+												○		+										2	2
10																																					0	0
11																					○	+															1	1
																																					37	34

cleaning actions: + this work; ○ Smaïli et al. BTA algorithm; ⊖ common

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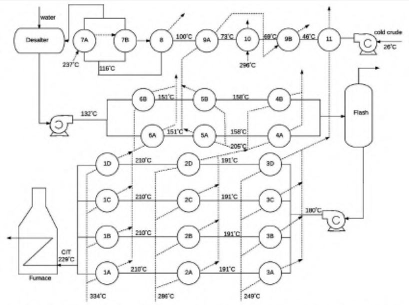

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1A												O					+								+	O											2	2
1B													+	O													⊖										2	2
1C												+	O												O	+											2	2
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2A										+					O								+				O										2	2
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2C														O		+								O			+										2	2
2D												+	O												⊖												2	2
3A																		+																			1	0
3B															+																						1	0
3C																	+	O																			1	1
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6A										O				+									O	+													2	2
6B															+			O					+														2	1
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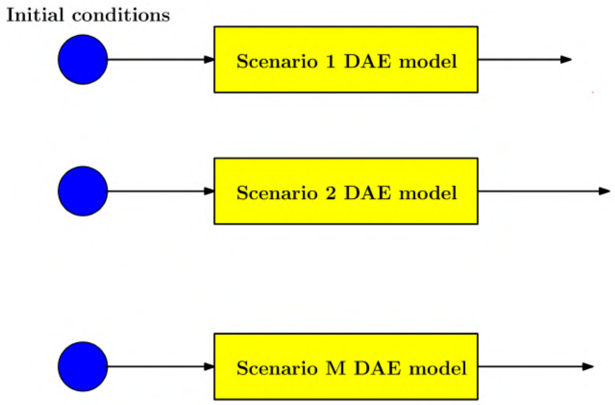
4/5: OCP under uncertainty (multiple scenario approach)



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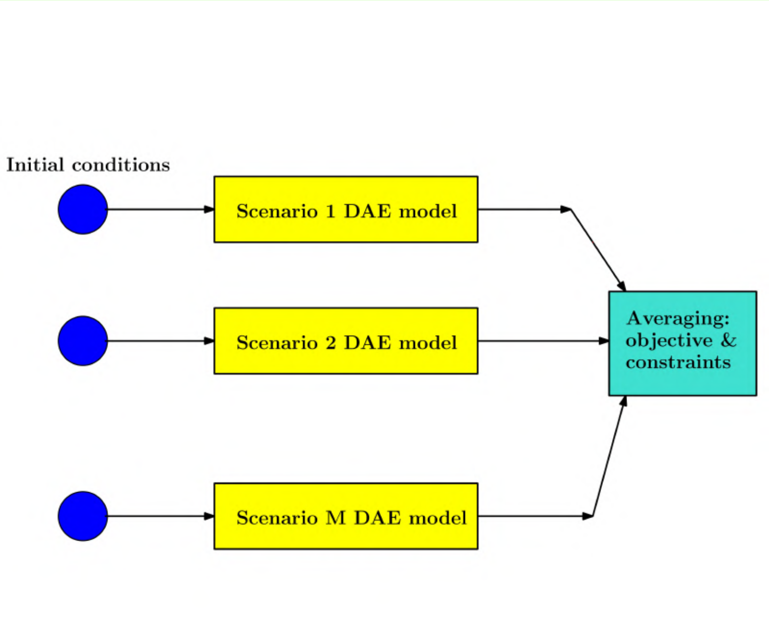

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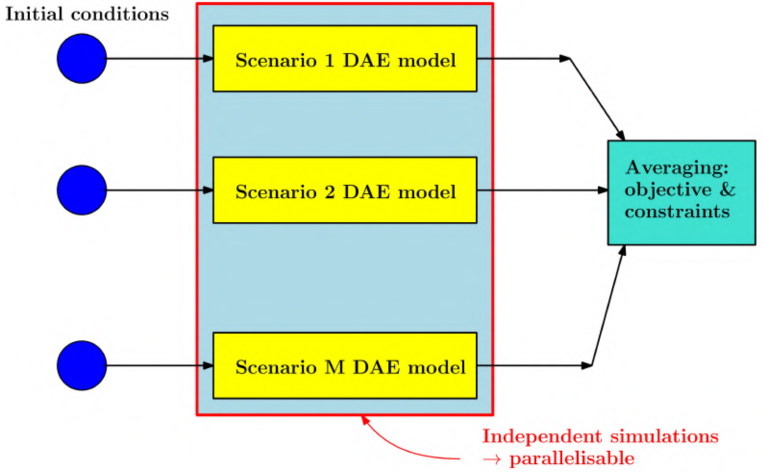

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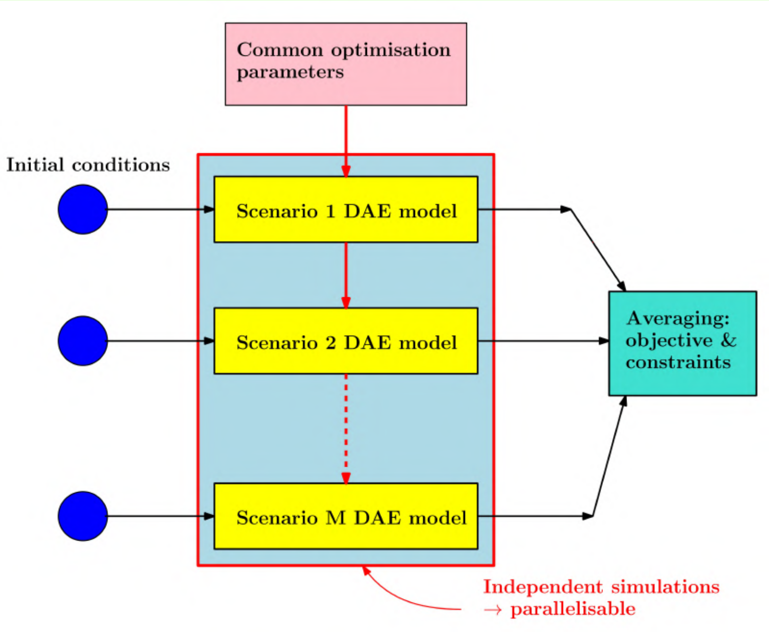

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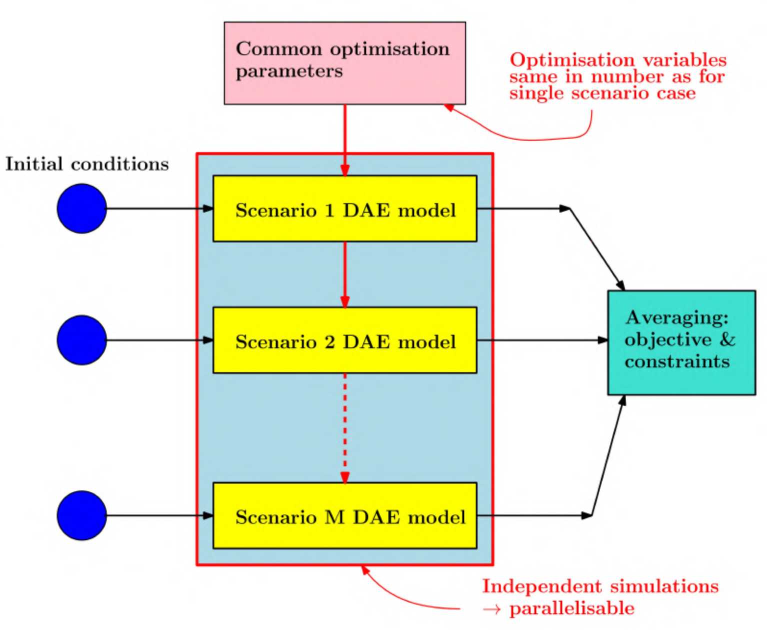

Application: maintenance scheduling of HENs subject to fouling[1]

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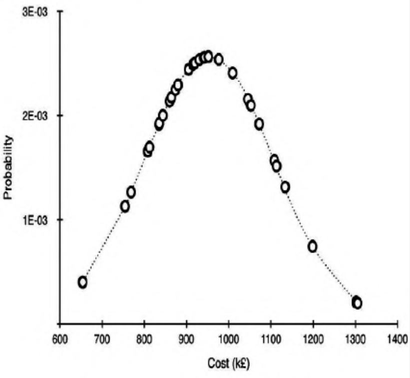

Fig. 6. Cost *versus* probability curve for Case II.

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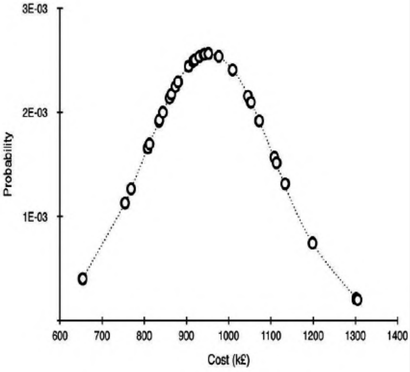

Fig. 6. Cost *versus* probability curve for Case II.

Table 19

Cleaning schedule for Case II with parametric uncertainty.

Time (months)

HEX	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
1A													O			+							+	O												
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4B												+				O								+		O										
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Cleaning actions: + parametric uncertainty case; O deterministic case; ⊕ common

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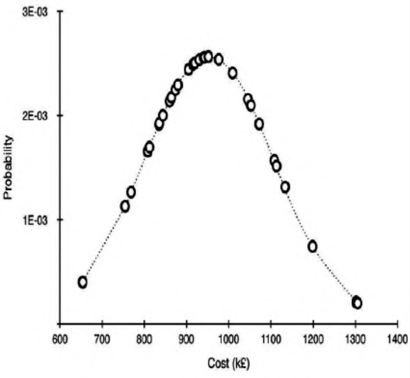

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5/5: Deterministic global optimisation of OCPs

- Methodology
  - overestimation of solution space of parameter-dependent ODEs
  - spatial B&B global optimisation algorithm
  - feasible path approach based methodology
- Contributions by Professor Claire Adjiman and coworkers[1,2]
- Contribution by Professor Paul Barton and coworkers[3]

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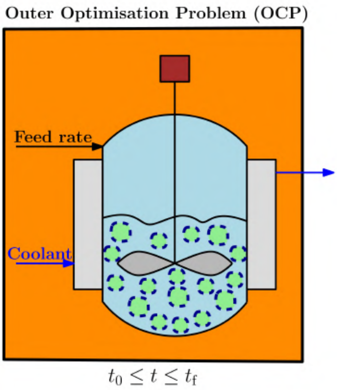
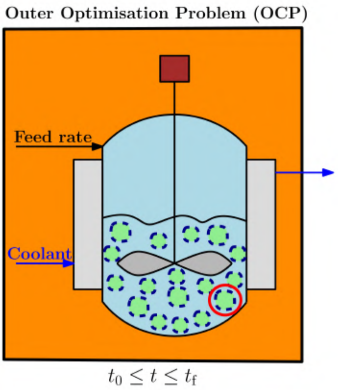
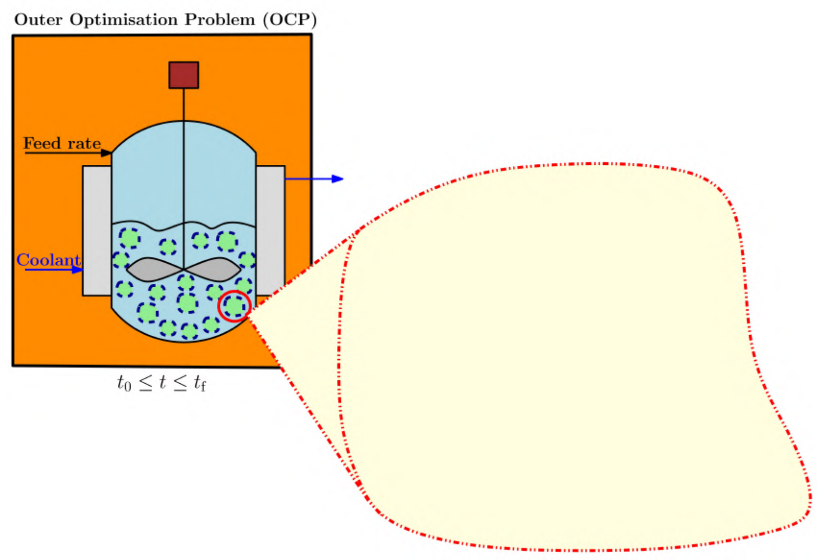
Outline

1/2: Dynamic biochemical processes, DFBA



1/2: Dynamic biochemical processes, DFBA




Outer Optimisation Problem (OCP)
Feed rate
Coolant
$t_0 \leq t \leq t_f$

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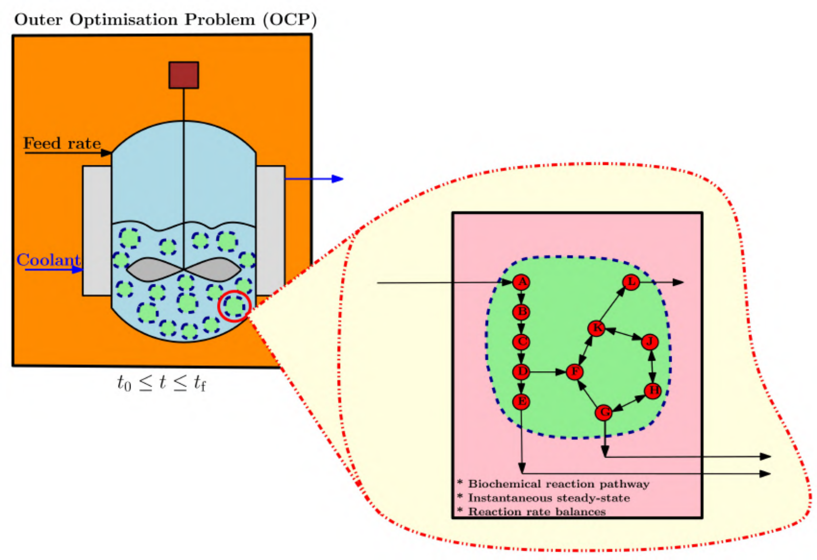
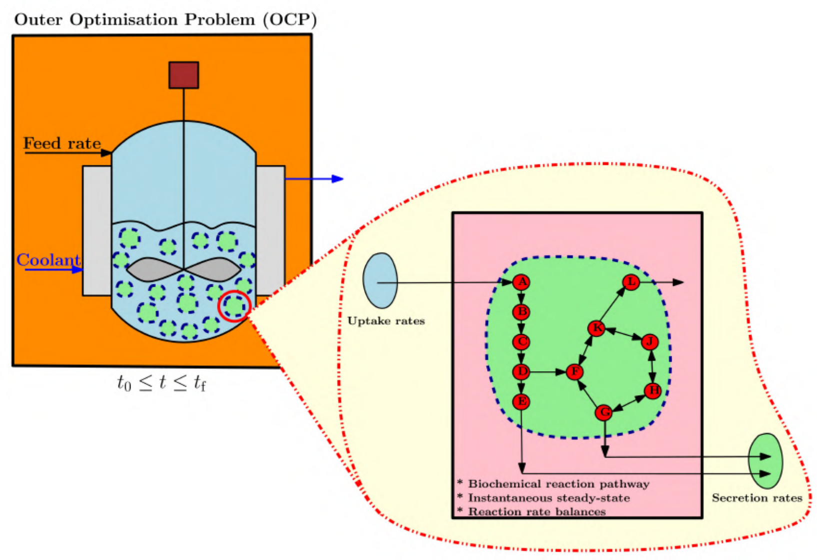
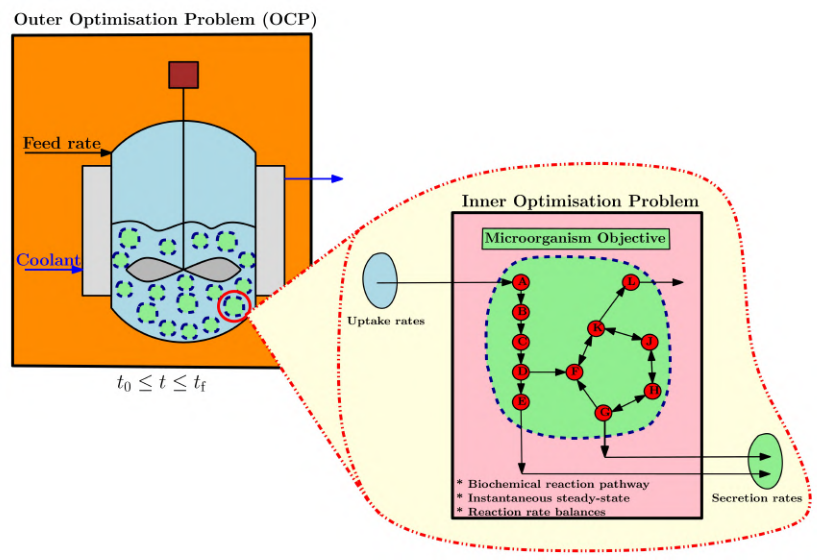
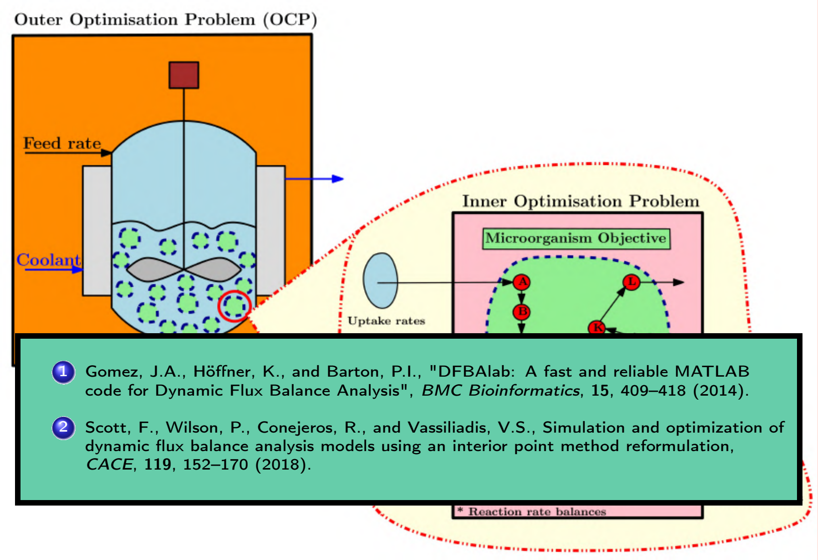



Outer Optimisation Problem (OCP)
Feed rate
Coolant
$t_0 \leq t \leq t_f$
Uptake rates
A
B
C
D
E
F
G
H
J
K
L
* Biochemical reaction pathway
* Instantaneous steady-state
* Reaction rate balances
Secretion rates

1/2: Dynamic biochemical processes, DFBA





1. Gomez, J.A., Höffner, K., and Barton, P.I., "DFBAlab: A fast and reliable MATLAB code for Dynamic Flux Balance Analysis", *BMC Bioinformatics*, **15**, 409–418 (2014).
2. Scott, F., Wilson, P., Conejeros, R., and Vassiliadis, V.S., Simulation and optimization of dynamic flux balance analysis models using an interior point method reformulation, *CACE*, **119**, 152–170 (2018).

2/2: Biomedical applications: towards personalised medicine

Example: scheduling drug treatments for the HIV infection[1]

- Validation and optimisation of Structured Treatment Interruptions (STI),
- Aim: suppress emergence of resistant mutations.

[1] Image from: Hadjiandreou, M.M., Conejeros, R., Vassiliadis, V.S., and Wilson, D.I., "Long-term HIV dynamics: Mathematical modelling and optimal control", Proc. Of the 2008 Int. Conf. on Bioinformatics and Computational Biology, BIOCOMP 2008 (2008).

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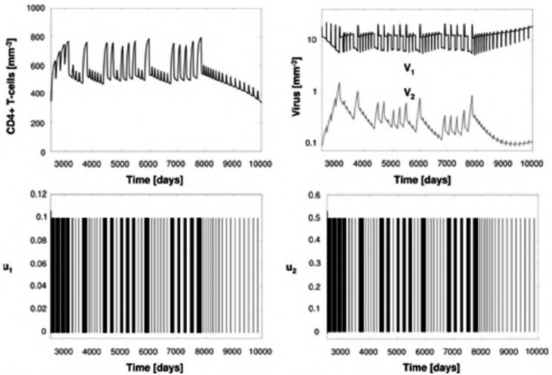

Fig. 5. Optimal control profiles (OCP2) of u_1 and u_2 for STIs for a Type I patient. Shaded region indicates treatment.

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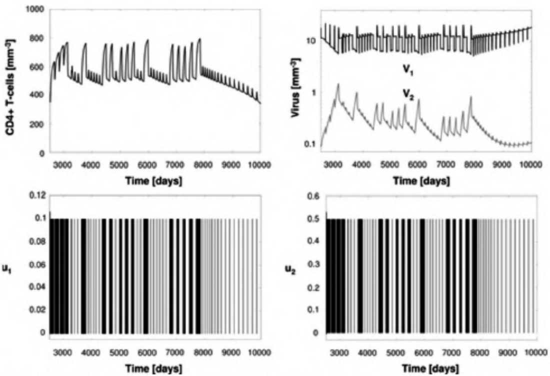

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Outline

In Prof.'s own words

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I hope that this cursory review has shown that there are still plenty of issues to address, and that there is an increasing range of techniques to do the job.

At CPSE, Imperial College London, circa 1990–1993

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R→L: Matheos, Vassilis, Lazaros

CPSE, 2nd floor, Imperial College London, circa 1990–1993

ESCAPE 3, Graz, Austria, 1993
R→L: Prof. Sargent, Thomas, Jorge, Vassilis

ESCAPE 3, Graz, Austria, 1993
R→L: Steve, Nilay, Prof. Sargent, Jorge, Stratos, Vassilis

PSE@Cambridge!

PSE@Cambridge!

Thank you all, and ...

... thank you, Prof.