COMPUTING IN CHEMICAL ENGINEERING:
Three decades in the development of algorithms and software

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MACHINE COMPUTATION COMMITTEE

• Formed in 1958
  – Computer program interchange
  – Publication of computer abstract programs

• Property estimation but lethargic in 1960s

• Charlie Ware led MCC’s rebirth in mid 1970s
  – 57 members in 1976; up from 34 in 1975
  – 8 computing sessions in 1976; up from 4 in 1975

• Questionnaires—Computing in the 1980s

• 1977 first issue of CACE (Dick Hughes)
  – Publishes “algorithms and programs” (Charlie Ware)
CAST division began operating in 1978
  – Technical Computation Newsletter of MCC becomes CAST Newsletter
  – 430 members joined in first year
  – What’s in a name?
    » Bob Morris

First CAST dinner in 1978
  – Stu Churchill
    » When is computing necessary?

“Computing in Chemical Engineering” award
  – First awarded to Dick Hughes in 1979
    » Computer or Engineer—Which is the boss?
ENABLING SOFTWARE—SIMULATION

• FLOWTRAN
  – Bob Seader
  – Monsanto launched it in 1966; sold outside in 1969
  – FLOWTRAN Simulation—An Introduction
  – Installed in over 150 universities (1988)

• ASPEN
  – Larry Evans with Paul Gallier, Herb Britt, Joe Boston, ...
  – DOE funding at MIT 1975-1981
  – Could not raise venture capital until 1986
  – Began penetrating mainstream 1986-1991
  – Initial public offering in 1994
  – Acquired over 20 companies
ENABLING SOFTWARE—OPTIMIZATION

• DICOPT
  – MINLP
  – Ignacio Grossmann
  – Planning, scheduling, design, synthesis
  – Under GAMS in 1990
    » Available to economists, OR analysts, ...

• SQP-rSQP-IPOPT
  – NLP
  – Larry Biegler
  – SQP codes powered FLOWTRAN and ASPEN
  – IPOPT is open source

• BARON
  – Global NLP and MINLP
MORE ENABLING SOFTWARE FROM CAST MEMBERS

• AIDES (Jeff Siirola and Dale Rudd)
MORE ENABLING SOFTWARE FROM CAST MEMBERS

- AIDES (Jeff Siirola and Dale Rudd)
- ASCEND (Art Westerberg)
- DESIGN-KIT, MODEL.LA, ...
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• DMC (Charlie Cutler)
• gPROMS (Costas Pantelides/PSE)
• OCTAVE (Jim Rawlings)
• POLYMATH (M. Cutlip and M. Shacham)
• SimuSolv (Gary Blow)
• SPEEDUP (Roger Sargent and Art Westerberg)
Classical optimization algorithms provide a local minimum "closest" to the starting point used.
Convexification

Range Reduction

Finiteness

BRANCH-AND-REDUCE

Students: Hong Ryoo, Joe Shectman, Vinay Ghildyal, Nilanjan Adhya, Mohit Tawarmalani, Xiaowei Bao, Aida Khajavirad, Keith Zorn
BARON SOFTWARE

• First commercial software to offer deterministic guarantee of global optimality for multi-extremal nonlinear optimization problems

• Two-pronged approach to technology transfer
  – Commercial
    » Under the modeling languages GAMS and AIMMS
  – Free
    » Under the NEOS server for optimization
BARON IN APPLICATIONS

• Development of new Runge-Kutta methods for partial differential equations

• Energy policy making

• Design of metabolic pathways
  – Grossmann, Domach and others, *Computers & Chemical Engineering*, 2005

• Model estimation and automatic control
  – Bemporand and Ljung, *Automatica*, 2004

• Agricultural economics
  – Cabrini *et al.*, *Manufacturing and Service Operations Management*, 2005
BIOINFORMATICS

Protein side-chain conformation prediction

Protein structure alignment

Students: Wei Xie, Shweta Shah
X-RAY CRYSTALLOGRAPHY

Algorithms in Hauptman’s Shake-and-Bake

Students: Anastasia Vaia, Alex Smith
PARALLEL COMPUTING WITH GRAPHICS PROCESSING UNITS
## GPU SPEEDUPS ACROSS FIELDS

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Field</th>
<th>Speedup</th>
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<td>CO$_2$ sequestration</td>
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<td>Computational finance</td>
<td>100x</td>
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<td>2-electron repulsion integral</td>
<td>Quantum chemistry</td>
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<tr>
<td>n-body dynamics</td>
<td>Astrophysics</td>
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<td>Simultaneous iterative reconstruction technique</td>
<td>Computer tomography</td>
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<tr>
<td>Euler solver</td>
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<td>SpMV (sparse)</td>
<td>Linear algebra</td>
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<td>Iterative linear algebra</td>
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<tr>
<td>BLAST</td>
<td>Bioinformatics</td>
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</tr>
</tbody>
</table>

Postdoc: Panos Vouzis
• Probabilistic and worst-case analysis of heuristics for process synthesis
  – Students: Ming-Long Liu, Shabbir Ahmed, Kevin Furman

• Heat exchanger network synthesis is “NP-hard in the strong sense”
  – Student: Kevin Furman

• Stochastic programming
  – Student: Shabbir Ahmed

• Supply chain management and design
  – Students: Ming-Long Liu, Shabbir Ahmed, Ramon Gutierrez
• Systems biology and bioinformatics
  – Students: YoungJung Chang, Saurabh Awasthi, Danan Wicaksono

• Portfolio optimization
  – Students: Luis Miguel Rios, Yizhi Zheng, Rohan Desai

• Energy systems modeling
  – Alison Cozad, Yan Zhang

• Molecular design
  – Students: Minrui Yu, Gautam Nanda, Apurva Samudra

• The time-dependent traveling salesman problem
  – Student: Russ Vander Wiel
OTHER WORK—Continued

• Successive linear programming
  – Student: Yiqi Zhu

• Integer programming
  – Students: Sumit Mehra, Mayank Mishra

• Linear programming
  – Students: Joe Elble, Deepak Channamariyappa

• Derivative-free optimization
  – Students: Luis Miguel Rios

• Machine learning
  – Students: Yannis Voudouris, Xuan Shi, Alison Cozad
AN UNEXPECTED CITATION

- Guide for amusement park patrons
- Acknowledgement for contributing “a number of exceptionally helpful studies”
- Park patrons measure satisfaction based on number of attractions they experience
- Minimize waiting time
- Waiting times depend on sequence and time of day
- Optimal tour: the time-dependent traveling salesman problem
  - Student: Russ Vander Wiel
  - Making polymers on continuous parallel lines …

http://touringplans.com/
CONCLUSIONS

• CAST members have produced software with tremendous impact
• Enabling technologies in simulation and optimization
• Impact across academic disciplines and areas well beyond chemical engineering
• Further advances in simulation and optimization are badly needed
• PSE activity in simulation and optimization will grow as use of computing in application areas increases
ACKNOWLEDGMENTS

• My former and current students
  – For all they have taught me
• Aristotle University of Thessaloniki
  – Costas Kiparissides
• Carnegie Mellon University
  – Larry Biegler
  – Ignacio Grossmann
  – Gary Powers
  – Art Westerberg
  – Erik Ydstie
• University of Illinois
  – Udatta Palekar
  – Arne Pearlstein
  – Chip Zukoski
• Colleagues
  – Manfred Morari
  – Costas Pantelides
  – Hanif Sherali
  – George Stephanopoulos
• CAST
• American Chemical Society
• CAPD
• Department of Energy
  – National Energy Technology Lab
• DuPont
• ExxonMobil
• Lucent Technologies
• Mitsubishi Chemicals
• National Institutes of Health
  – General Medical Sciences
• National Science Foundation
  – Bioengineering and Environmental Sciences
  – Chemical and Thermal Systems
  – Design and Manufacturing
  – Electrical and Communication Systems
  – Operations Research
• Swearingen Chair
• TAPPI
• Univ. of Illinois Research Board