Interior Point Algorithms for Large-Scale Nonlinear Programming: Applications in Dynamic Systems

L. T. Biegler
Chemical Engineering Department
Carnegie Mellon University
Pittsburgh, PA

March, 2005

Overview

Introduction

- NLP Formulation for Dynamic Systems

Large Scale NLP for Dynamic Systems

- Flight Path Trajectory Planning and Control
- Grade Transitions for Polymerization Processes

Optimization Models with Complementarity Constraints

- Metabolic Flux Balances for Yeast Fermentation

Conclusions

Dynamic Optimization Problem

$$\min \psi \left(z(t),\ y(t),\ u(t),\ p,\ t_f\right)$$

s.t.

$$\frac{dz(t)}{dt} = F\left(z(t), y(t), u(t), t, p\right)$$

$$G\left(z(t), y(t), u(t), t, p\right) = 0$$

$$z^o = z(0)$$

$$z^l \le z(t) \le z^u$$

$$y^l \le y(t) \le y^u$$

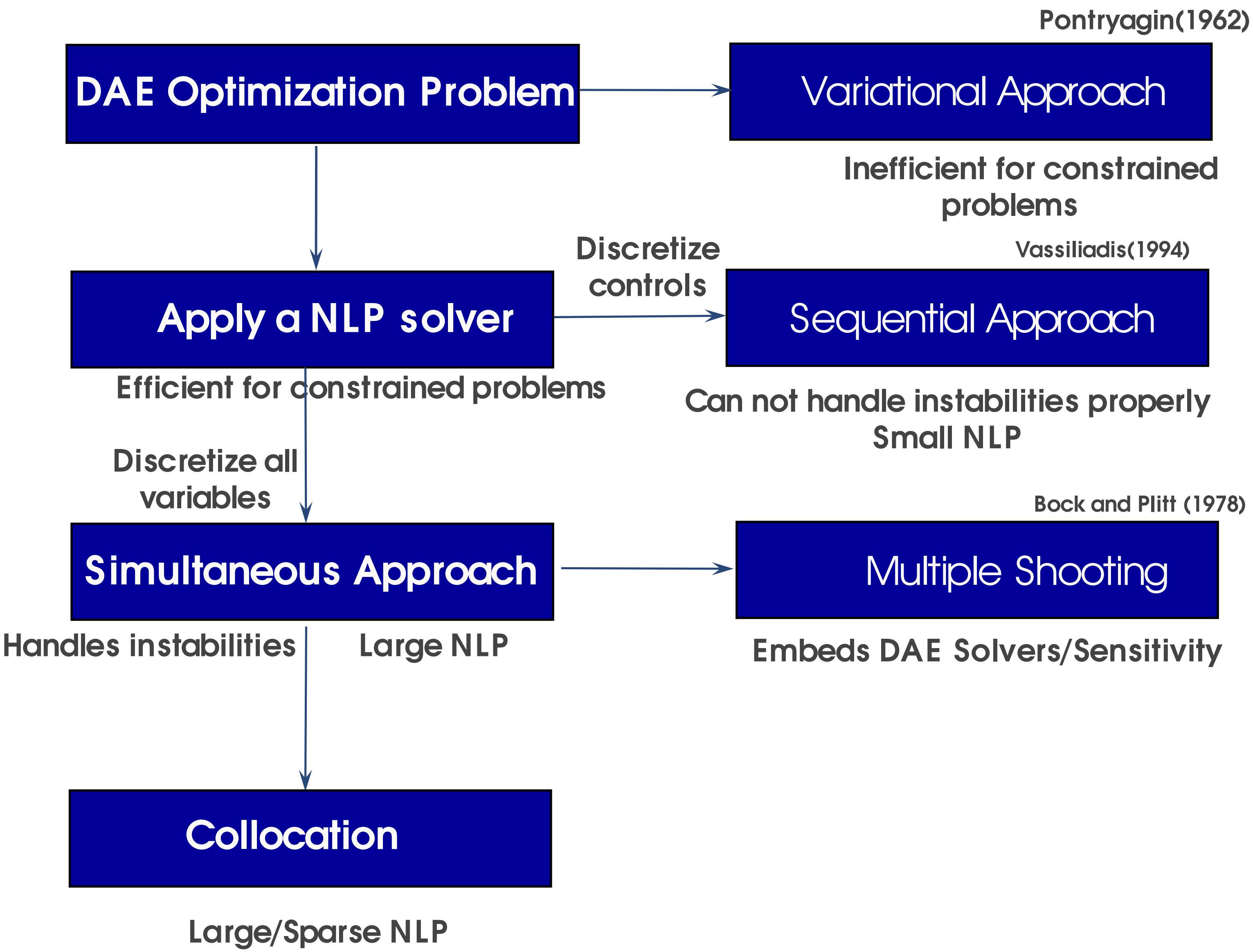
$$u^l \le u(t) \le u^u$$

$$p^l \le p \le p^u$$

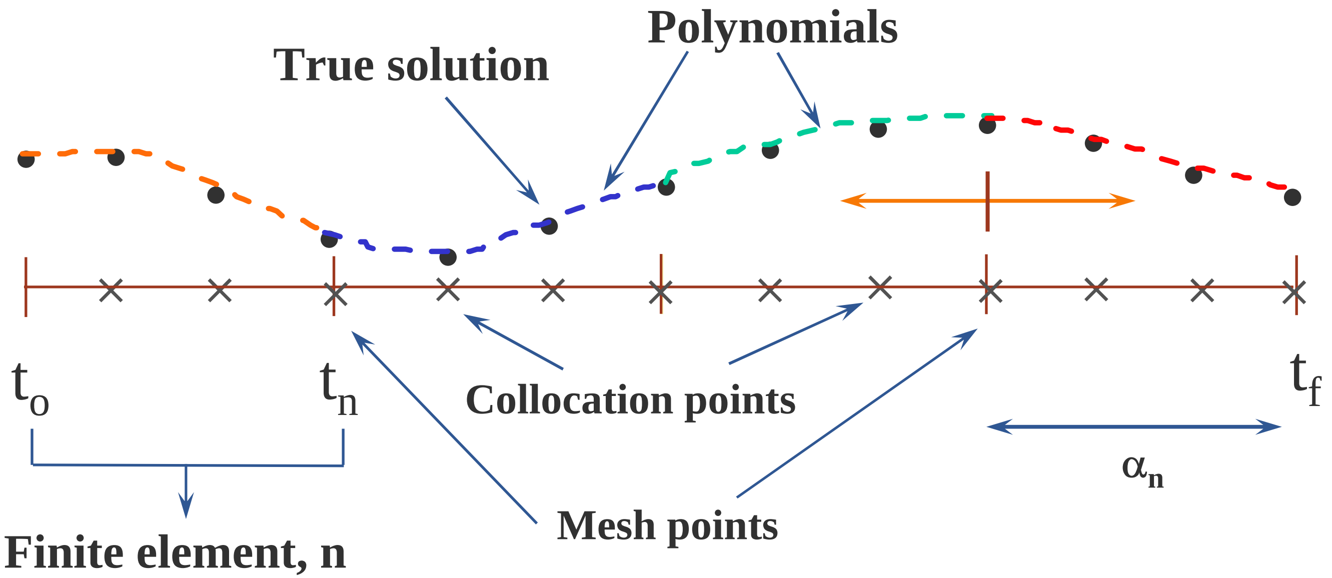
t, time
z, differential variables
y, algebraic variables

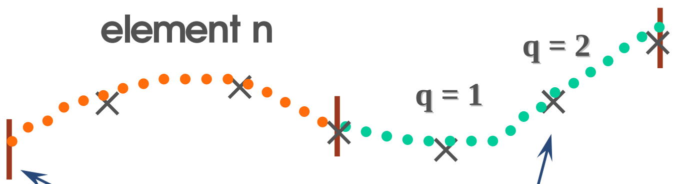
t_f, final time
u, control variables
p, time independent parameters

Dynamic Optimization Approaches



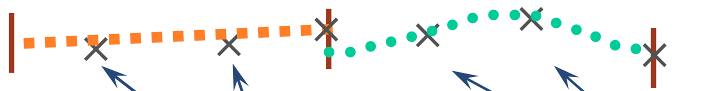
Collocation on Finite Elements





$$z(t) = z_{n-1} + (t - t_{n-1}) \sum_{q=1}^{k} g^q(t) \frac{dz^q}{dt}_n$$

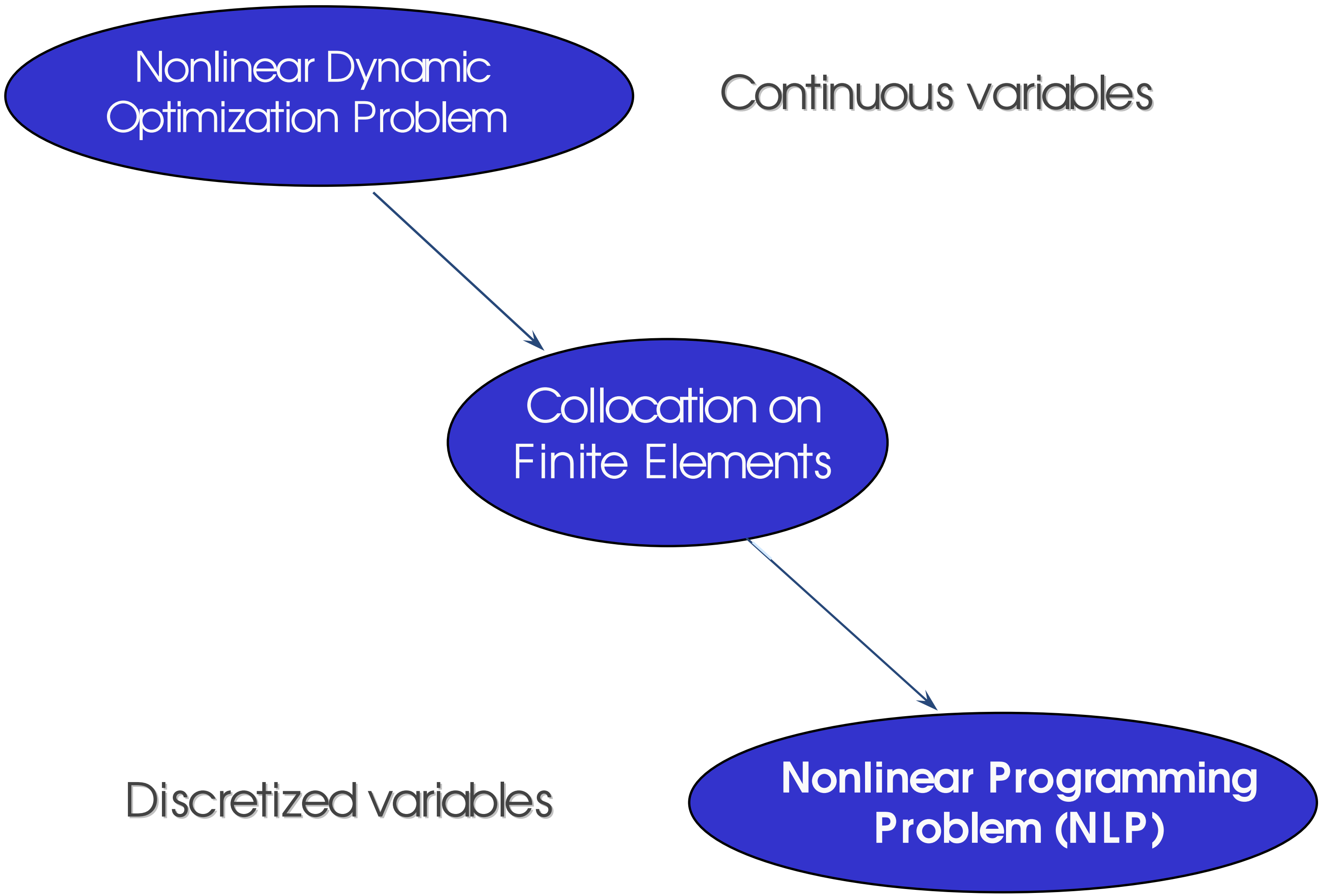
Differential variables
Continuous



$$y(t) = \sum_{q=1}^{k} g^q(t) y_n^q \qquad u(t) = \sum_{q=1}^{k} g^q(t) u_n^q$$

Algebraic and
Control variables
Discontinuous

Nonlinear Programming Formulation



Nonlinear Programming Problem

$$\min \psi\left(z_i, y_{i,q}, u_{i,q}, p, t_f\right)$$

s.t. $$\left(\frac{dz}{dt}\right)_{i,j} = F\left(z_{i-1}, \frac{dz}{dt}_{i,j}, z_i, y_{i,j}, u_{i,j}, p\right)$$

$$G\left(z_{i-1}, \frac{dz}{dt}_{i,j}, z_i, y_{i,j}, u_{i,j}, p\right) = 0$$

$$z_i = f\left(\frac{dz}{dt}_{i-1,j}, z_{i-1}\right)_i$$

$$z_0^o = z(0)$$

$$z_i^l \le z_i \le z_i^u$$

$$y_{i,j}^l \le y_{i,j} \le y_{i,j}^u$$

$$u_{i,j}^l \le u_{i,j} \le u_{i,j}^u$$

$$p^l \le p \le p^u$$

$$\min_{x \in \Re^n} f(x)$$

$$\text{s.t} \quad c(x) = 0$$

$$a \le x \le b$$

Simultaneous Dynamic Optimization (Direct Transcription)

Advantages

- Equivalence of NLP solutions and Euler-Lagrange conditions
- Convergence rates to Euler-Lagrange conditions
- Treatment of open-loop unstable systems
- Treatment of path constraints
- Exploit sparsity and structure

Challenges

- Accurate state and control profiles
  - Moving finite elements
  - Formulations with embedded error criteria
- Solution of large-scale NLPs

Large Scale NLP Algorithms

Motivation: Improvement of Successive Quadratic Programming as Cornerstone Algorithm

➔ ***process optimization for design, control and operations***

Evolution of NLP Solvers:

SQP → rSQP → IPOPT

rSQP++

1999-02: Simultaneous dynamic optimization
over 1 000 000 variables and constraints

Current: Tailor structure, architecture and problems

IPOPT Algorithm – Features

Line Search Strategies for Globalization

- ℓ_2 exact penalty merit function
- augmented Lagrangian merit function
- **Filter method (adapted and extended from Fletcher and Leyffer)**

Hessian Calculation

- BFGS (full/LM and reduced space)
- SR1 (reduced space)
- **Exact full Hessian (direct)**
- Exact reduced Hessian (direct)
- Preconditioned CG

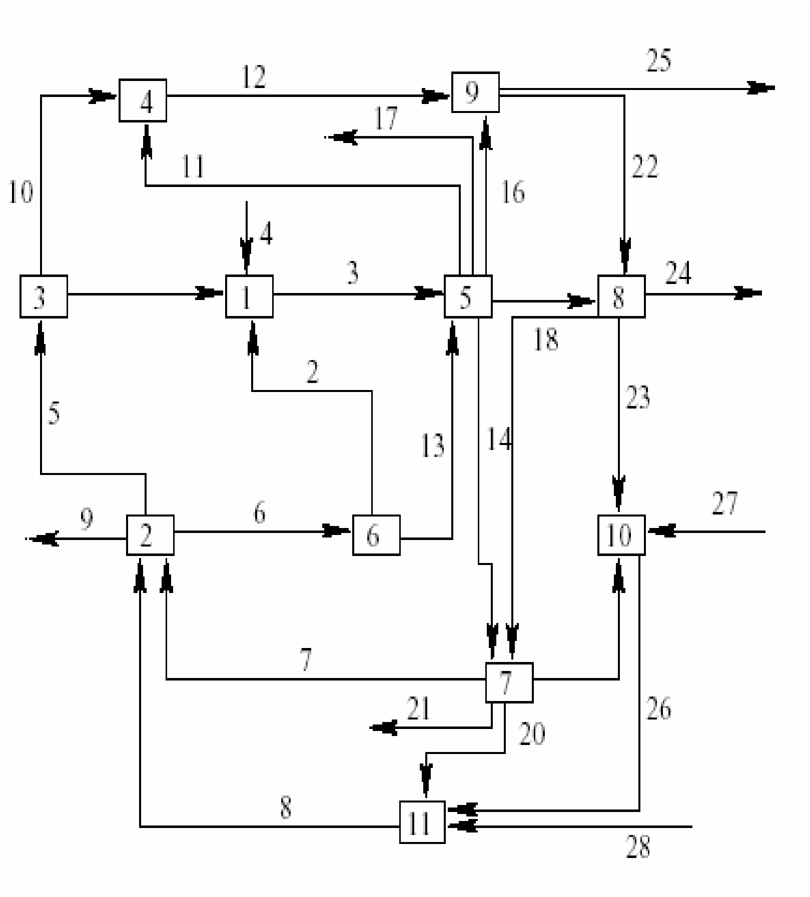
Algorithmic Properties

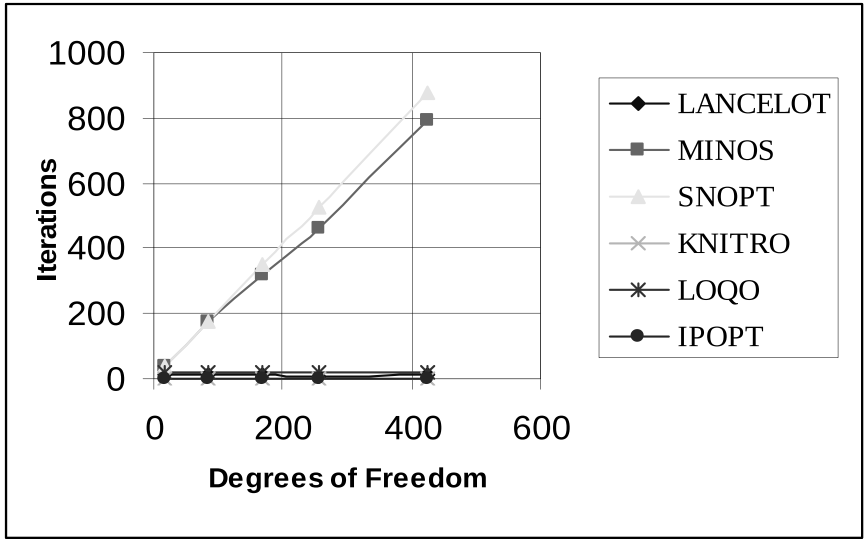
- **Globally and superlinearly convergent** (see Wächter and B., 2005a,b,c)
- Weaker assumptions than other codes
- Easily tailored to different problem structures

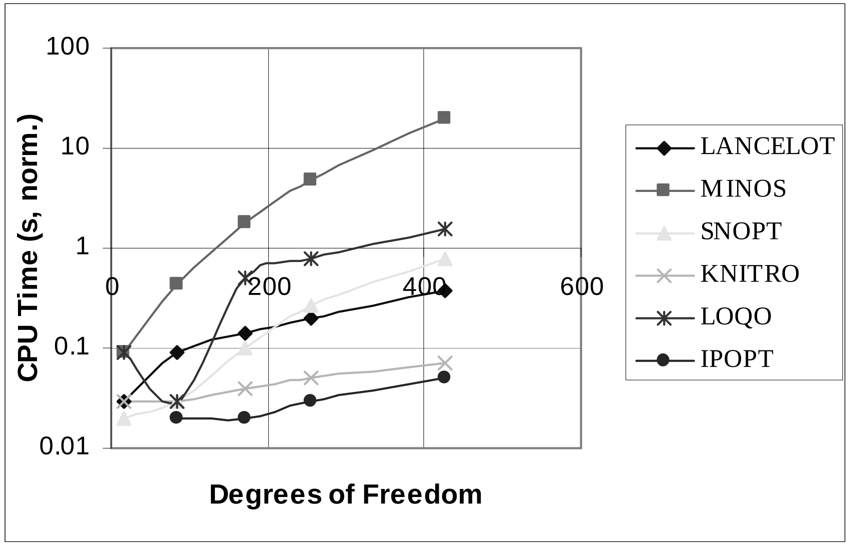
Freely Available

- CPL License and COIN-OR distribution
- new version recently rewritten in C++
- Solved on thousands of test problems and applications
- **Code avaliable at http://www.coin-or.org**

Comparison of NLP Solvers: Data Reconciliation
(Poku, Kelly, B. (2004))







Air Traffic Control – 3D Conflict Resolution

(Raghunathan et al., (2004)

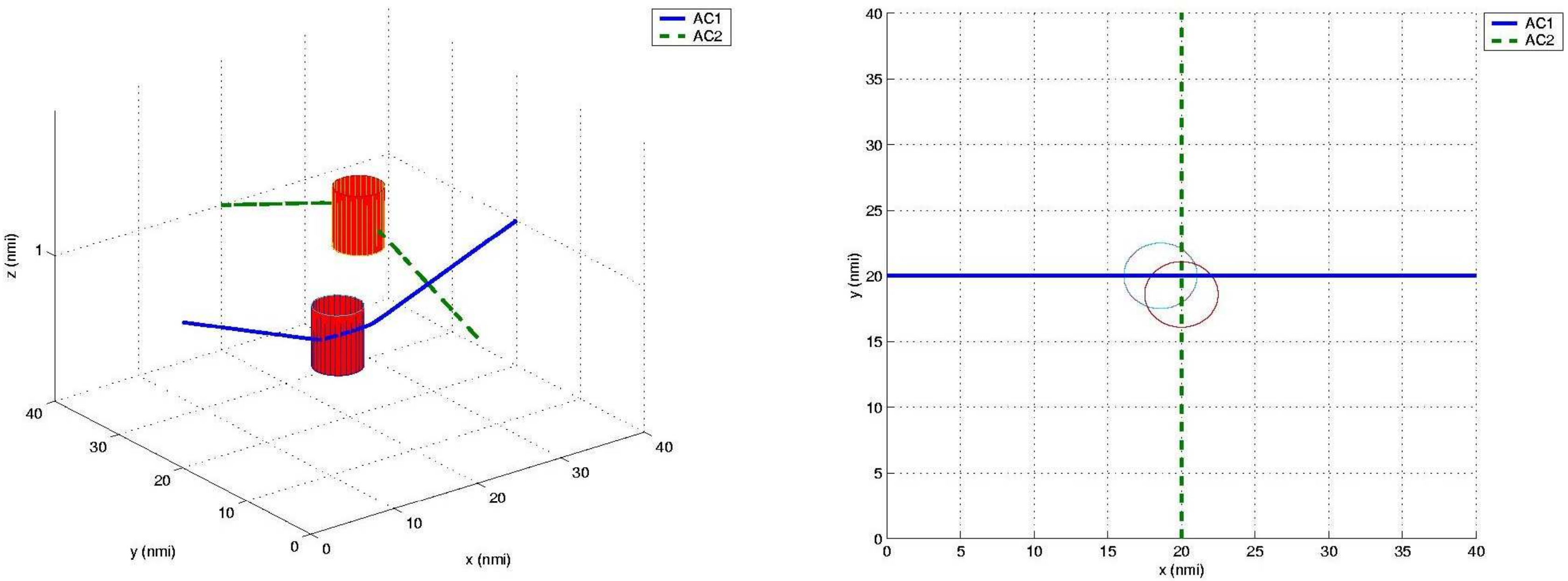


Figure 1: Three dimensional and top view of an optimal resolution maneuver for an orthogonal two-aircraft encounter ($\eta = 15$ and $\mu_1 = \mu_2 = 0.5$).

Air Traffic Control – Simple Kinematic Model

$$\min \quad \sum_{i=1}^{n} \mu_i J_i(v_{x,i}, v_{y,i}, v_{z,i})$$

s.t.

Equations of Motion

$$\frac{dx_i}{dt} = v_{x,i}(t); \quad x_i(t_0) = x_{i,0}; \quad x_i(t_f) = x_{i,f} \qquad i = 1, \ldots, n$$
$$\frac{dy_i}{dt} = v_{y,i}(t); \quad y_i(t_0) = y_{i,0}; \quad y_i(t_f) = y_{i,f} \qquad i = 1, \ldots, n$$
$$\frac{dz_i}{dt} = v_{z,i}(t); \quad z_i(t_0) = z_{i,0}; \quad z_i(t_f) = z_{i,f} \qquad i = 1, \ldots, n$$

Protection Zone

$$(x_i(t) - x_j(t))^2 + (y_i(t) - y_j(t))^2 \geq R^2 \vee |z_i - z_j(t)| \geq H \qquad i, j = 1, \ldots, n, i \neq j.$$

where:

$$J(v_x, v_y, v_z) = \frac{1}{2} \int [(v_x(t))^2 + (v_y(t))^2 + \eta^2 (v_z(t))^2] dt$$

Note nonconvexity in constraints

Air Traffic Control – Point Mass Model Detailed Flyability Behavior

Equations of Motion

$$\frac{dx_i}{dt} = V_i \cos\gamma_i \cos\chi_i \quad ; \quad x_i(t_0) = x_{i,0}; \quad x_i(t_f) = x_{i,f}$$

$$\frac{dy_i}{dt} = V_i \cos\gamma_i \sin\chi_i \quad ; \quad y_i(t_0) = y_{i,0}; \quad y_i(t_f) = y_{i,f}$$

$$\frac{dz_i}{dt} = V_i \sin\gamma_i \quad ; \quad z_i(t_0) = z_{i,0}; \quad z_i(t_f) = z_{i,f}$$

Detailed Flight Equations

$$\frac{dV_i}{dt} = \frac{T_i - D_i}{m_i} - g\sin\gamma_i \quad ; \quad V_i(t_0) = V_{i,0}$$

$$\frac{d\gamma_i}{dt} = \frac{g}{V_i}\left(\frac{L_i \cos\phi_i}{g m_i} - \cos\gamma_i\right); \quad \gamma_i(t_0) = \gamma_{i,0}$$

$$\frac{d\chi_i}{dt} = \frac{L_i \sin\phi_i}{m_i V_i \cos\gamma_i}; \quad \chi_i(t_0) = \chi_{i,0}$$

Protection Zone

$$|z_i(t) - z_j(t)| \geq H \quad \vee \quad (x_i(t) - x_j(t))^2 + (y_i(t) - y_j(t))^2 \geq R^2 \quad j = 1, \ldots, n, i \neq j$$

Flyability Constraints

$$D_i(t) = 0.01\rho_{\text{air}}(V_i(t))^2 S_i + \frac{0.6(L_i(t))^2}{\rho_{\text{air}}(V_i(t))^2 S_i}$$

$$V_{i,\min} \leq V_i(t) \leq V_{i,\max} \qquad |\phi_i(t)| \leq \phi_{i,\max}$$

$$0 \leq T_i(t) \leq T_{i,\max} \qquad 0 \leq L_i(t) \leq L_{i,\max}$$

ATC - 8 Aircraft
Detailed Point Mass Models

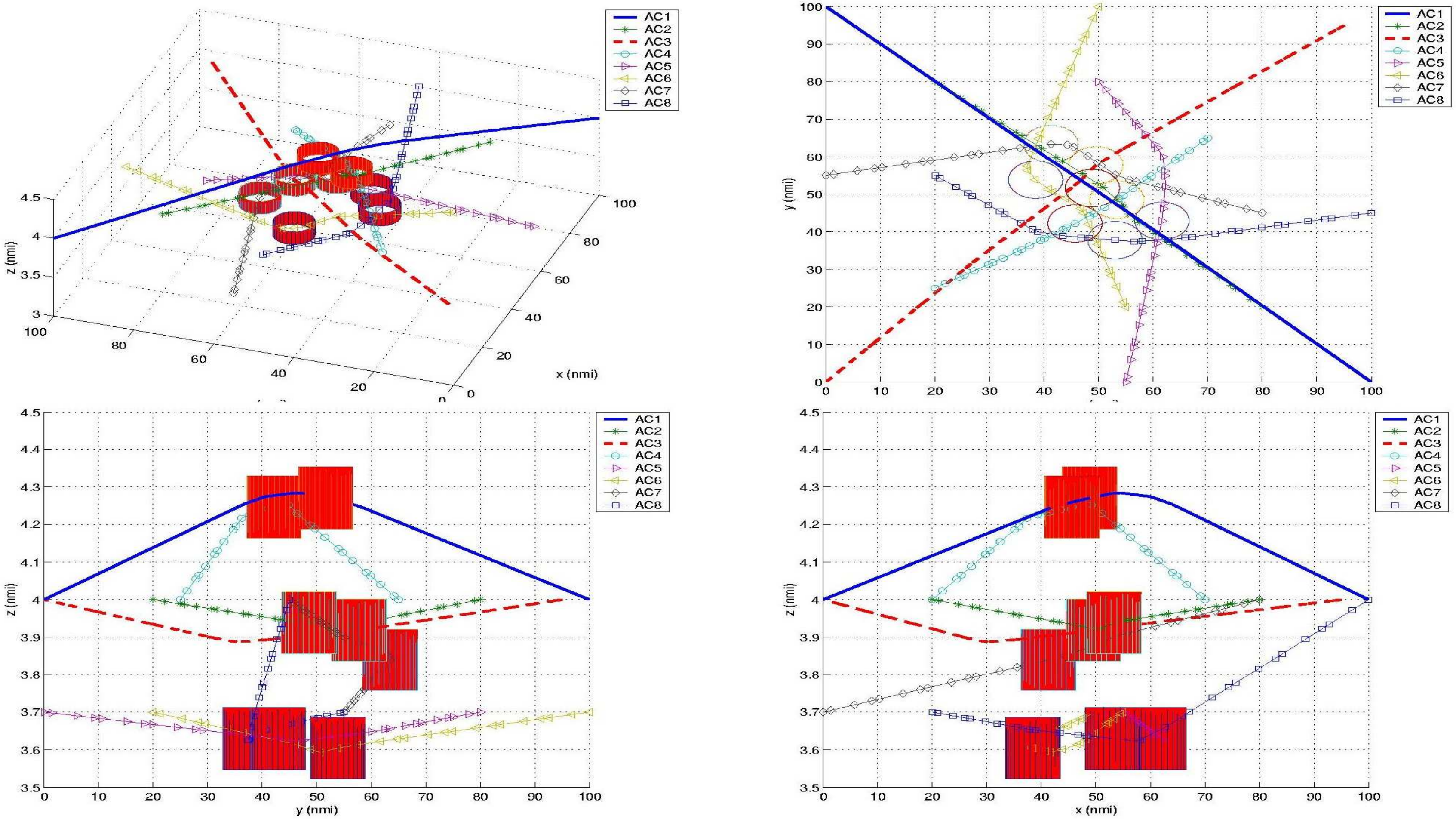
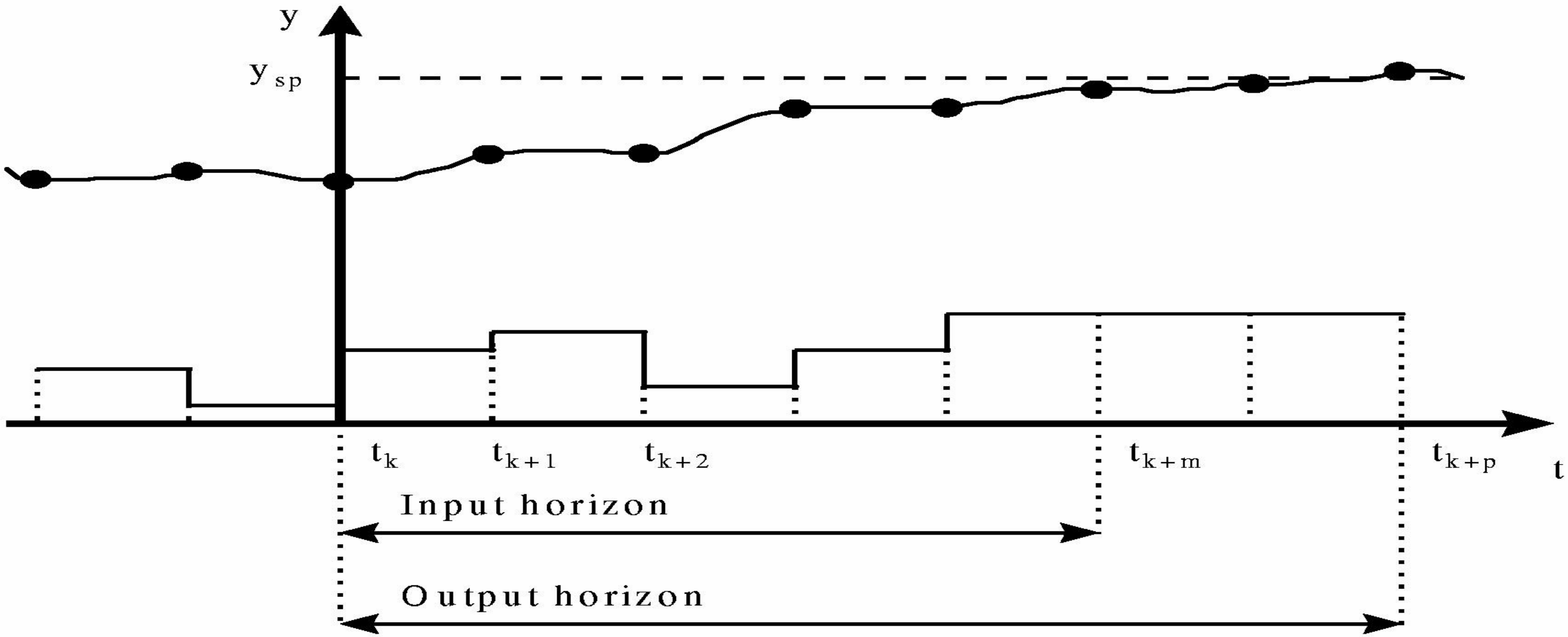


Figure 4: Optimal resolution maneuver for eight-aircraft encounter ($\eta = 20, \mu_i = 1/8, i = 1, \ldots, 8$).

Nonlinear Model Predictive Control (NMPC)

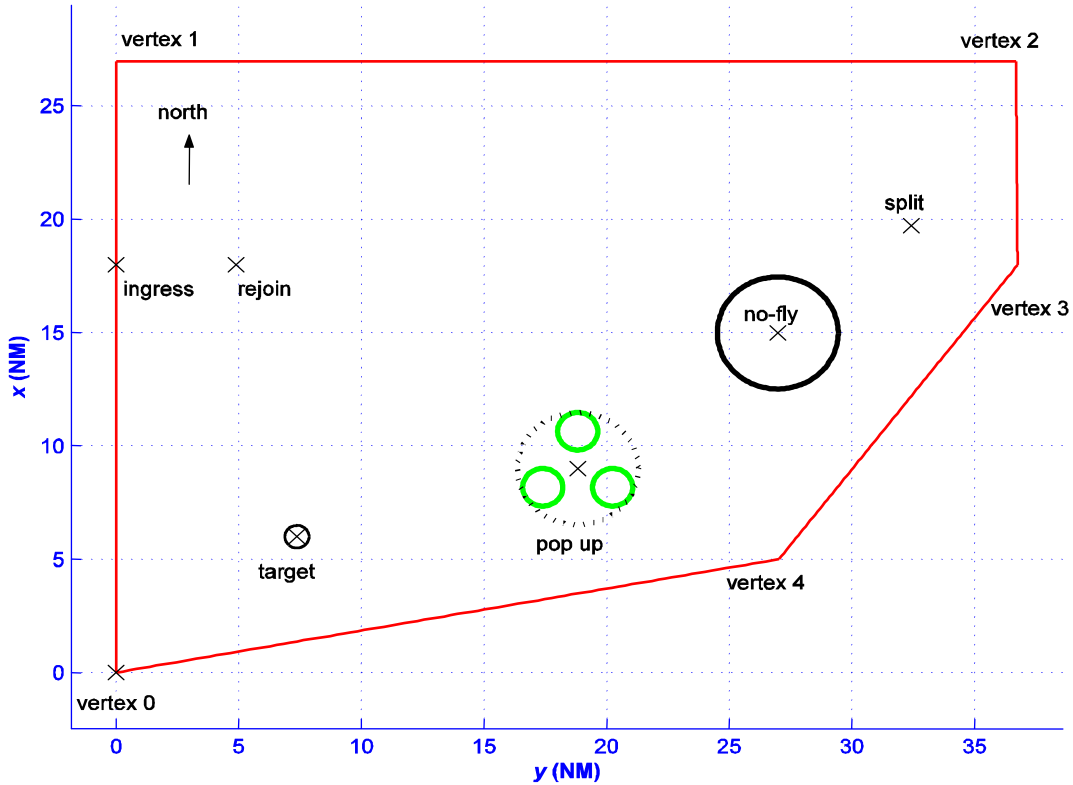


$$\min_{\boldsymbol{u}} \quad \sum \| y(t) - y^{\text{sp}} \|_{Q^y} + \sum \| \boldsymbol{u}(\boldsymbol{t}^k) - \boldsymbol{u}(\boldsymbol{t}^{k-1}) \|_{Q^u}$$

$$s.t. \quad \begin{aligned} & z'(t) = F(z(t), y(t), \boldsymbol{u}(t), t) \\ & 0 = G(z(t), y(t), \boldsymbol{u}(t), t) \\ & z(t) = z^{\text{init}} \\ & \text{Bound Constraints} \\ & \text{Other Constraints} \end{aligned}$$

Multi-stage ATC Problems in Real Time

Case study submitted by industry (Honeywell-DARPA)



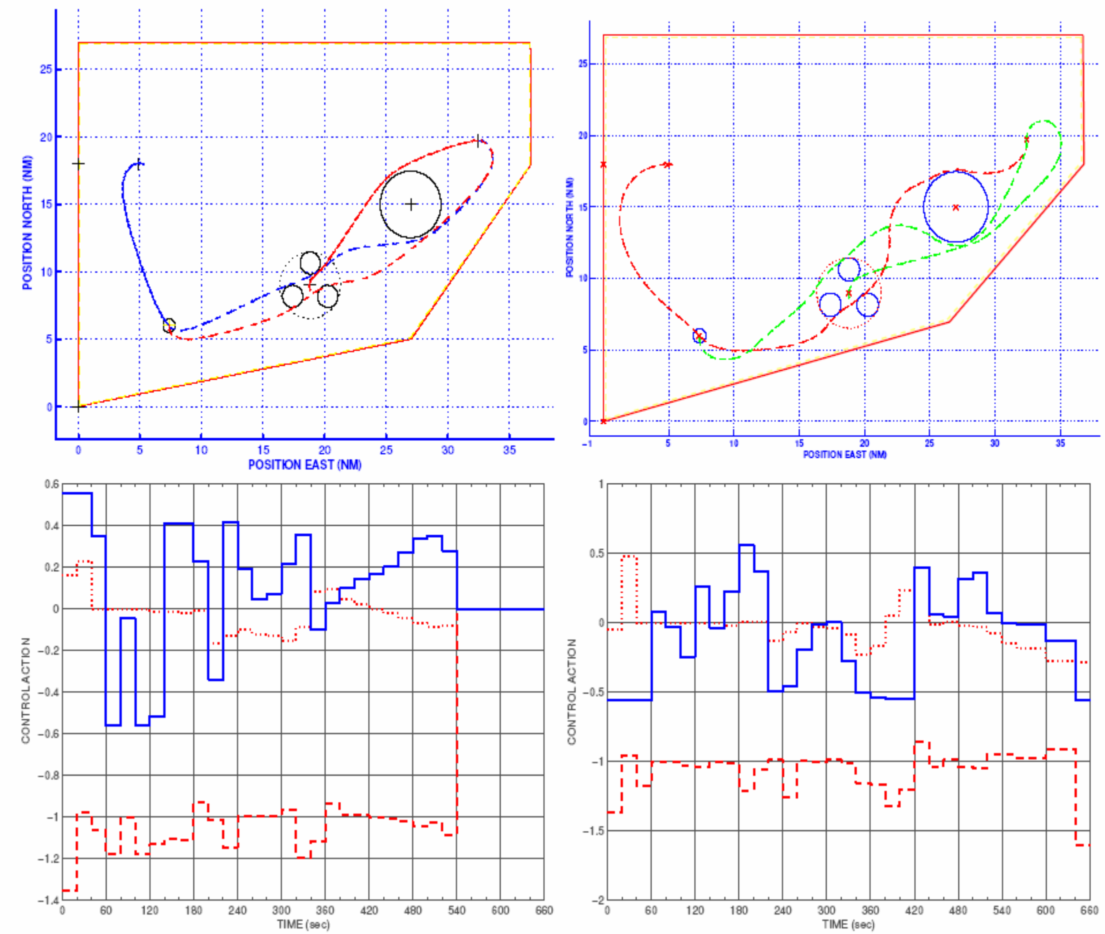
Cooperative T33 Aircraft

$$
\begin{aligned}
\dot{x} &= v \cos\gamma \cos\chi \\
\dot{y} &= v \cos\gamma \sin\chi \\
\dot{h} &= v \sin\gamma \\
\dot{v} &= g\,(n_x - \sin\gamma) \\
0 &= (v\dot{\chi}\cos\gamma)\cos\phi \\
&\quad - (v\dot{\gamma} + g\cos\gamma)\sin\phi \\
-n_h g &= (v\dot{\chi}\cos\gamma)\sin\phi \\
&\quad + (v\dot{\gamma} + g\cos\gamma)\cos\phi
\end{aligned}
$$

Task	Waypoint Agent 1	Waypoint Agent 2
Begin	rejoin	target
Mission 1	target	split
Mission 2	split	pop-up

NMPC Results for Multi-stage ATC

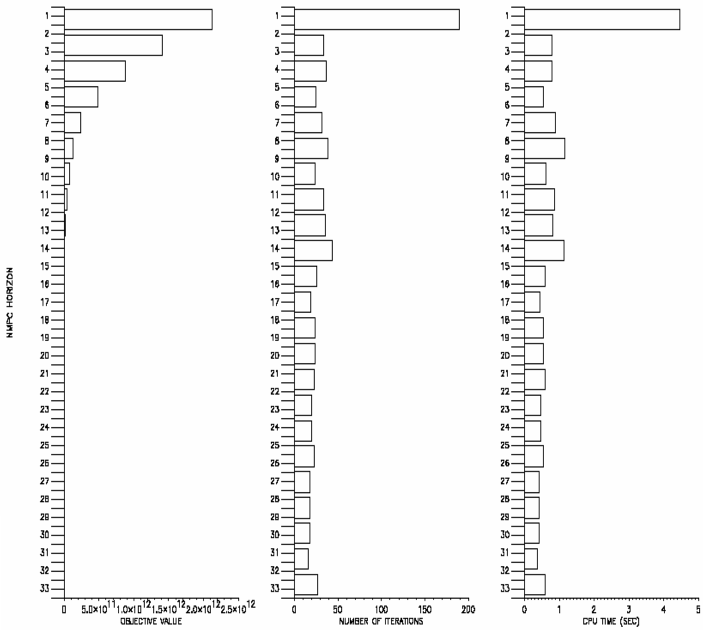
A full time solution was computed for comparison purposes.



Full time solution

- **1807** variables
- **1546** constraints
- **85.2** CPU seconds

NMPC solution



Applications of Simultaneous Dynamic Optimization (http://dynopt.cheme.cmu.edu)

Startup and Transient Operation

- Grade changes in LDPE processes
- Startup of Cryogenic Separation Processes
- Startup of unstable polymerization reactors
- Direct methanol fuel cell operation

Batch Process Operation

- Batch process operation of polymeric systems
- Batch distillation for brandy manufacture

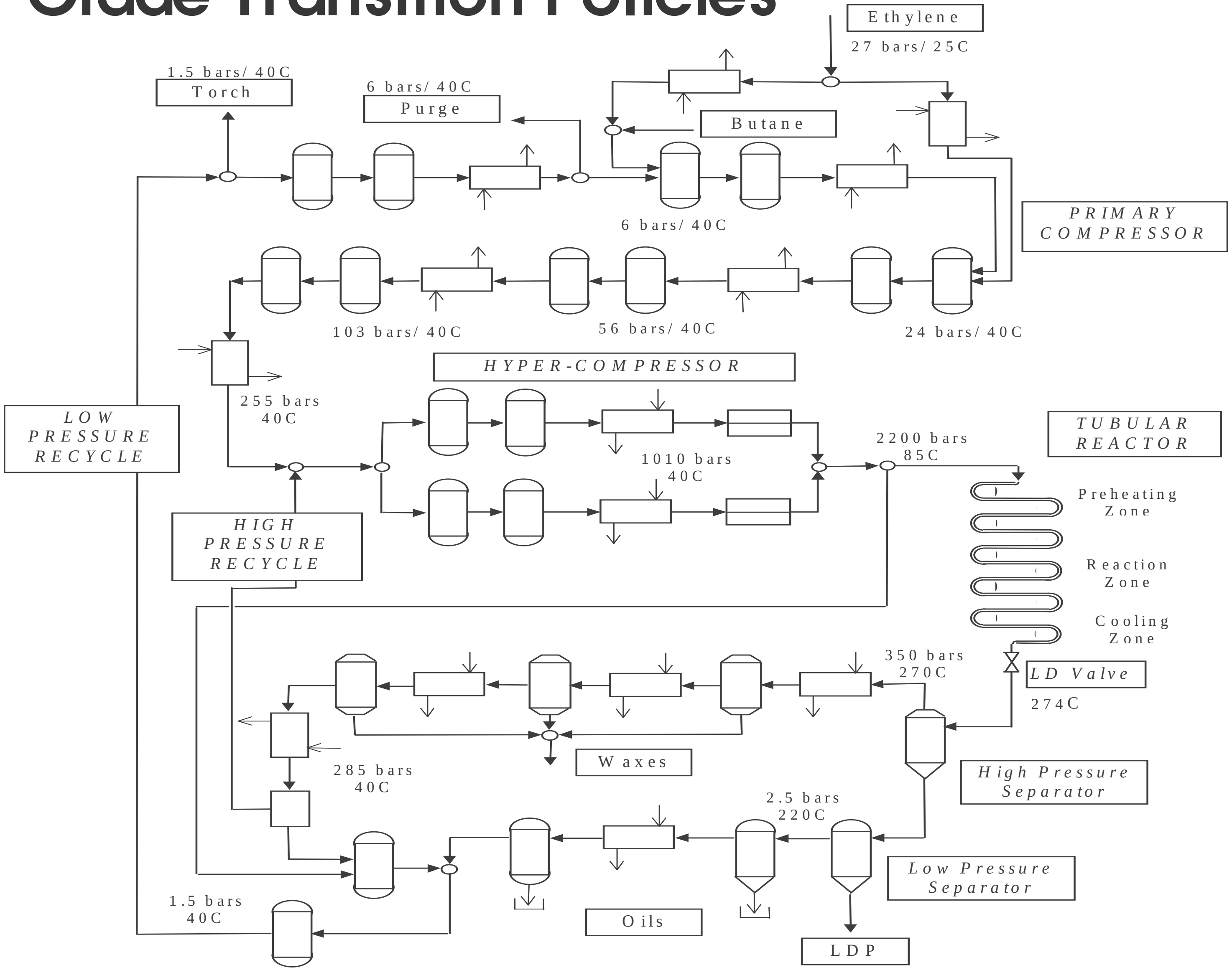
Design of Periodic Adsorption Systems

- Pressure Swing Adsorption
- Simulated Moving Beds

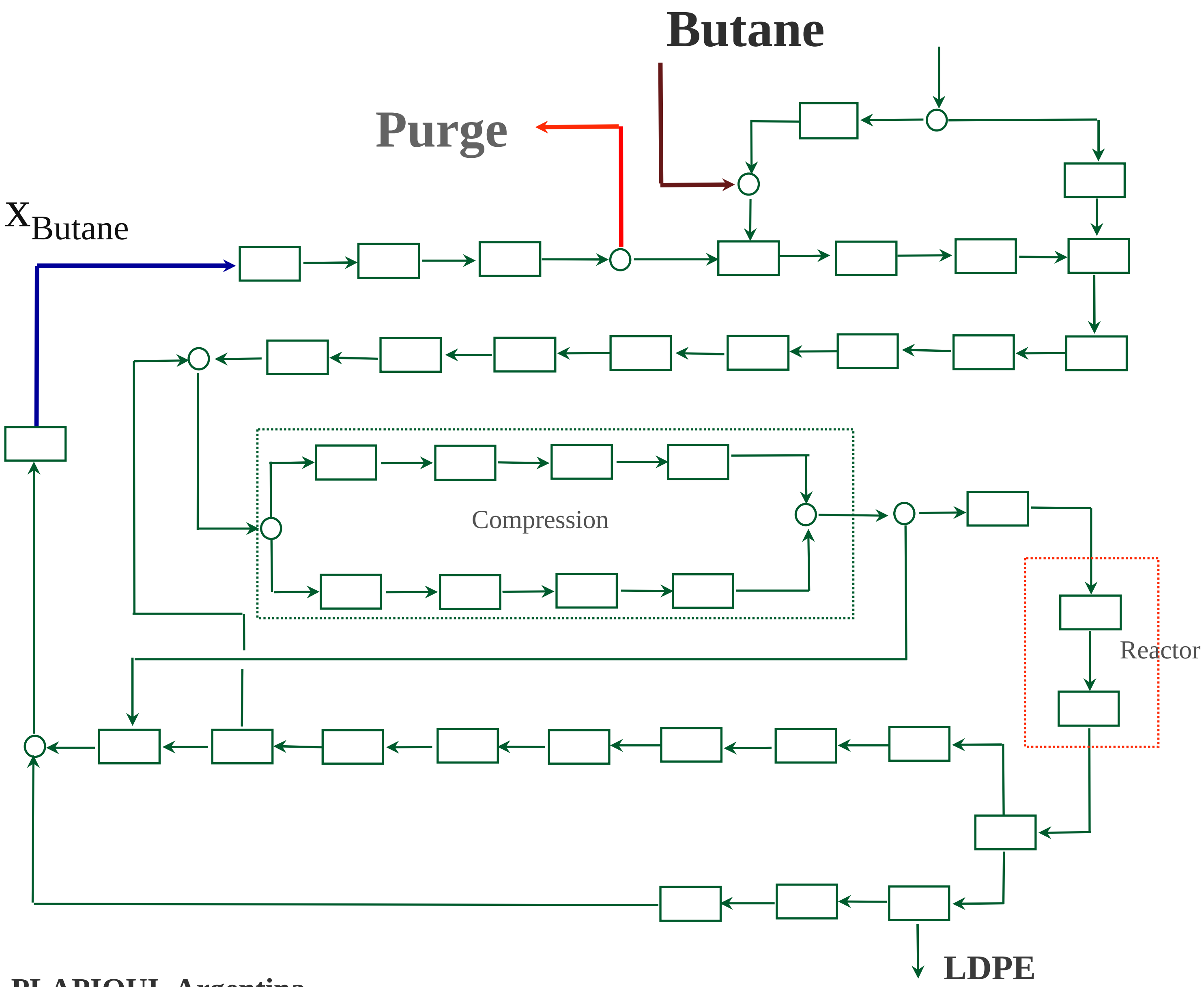
Parameter Estimation

- Batch polymerization reactors
- Direct methanol fuel cell operation
- Source inversion for municipal water networks

Low Density Polyethylene Plant Grade Transition Policies

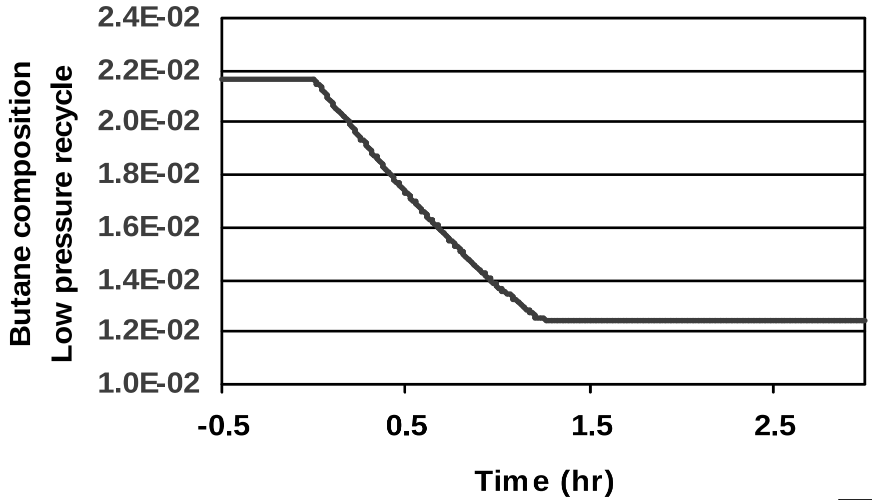


Low Density Polyethylene Plant

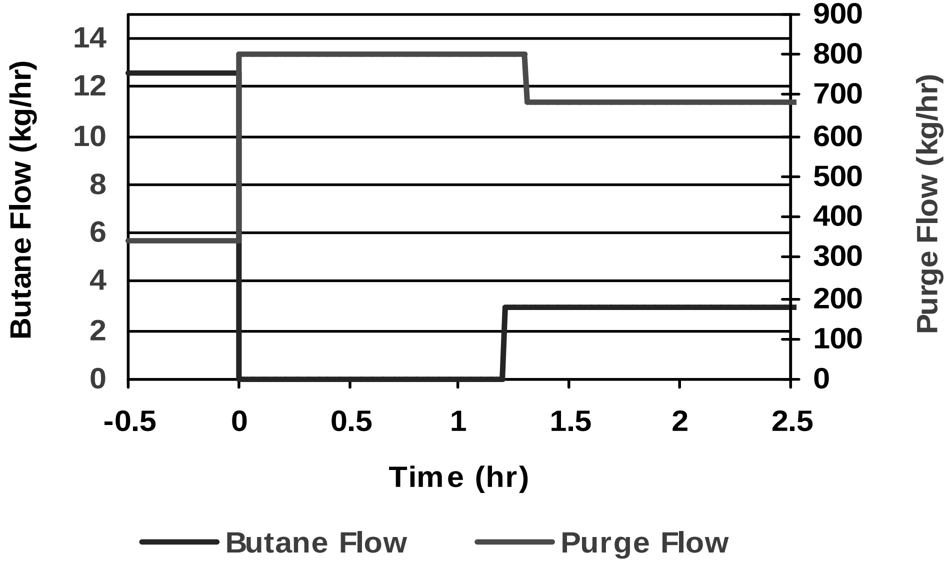


Low Density Polyethylene Plant
Simple Reactor Model

Increase the molecular weight



- **220 DAEs**
- **15 elements**
- **3 collocation points**
- **684.72 CPU s (P3)**

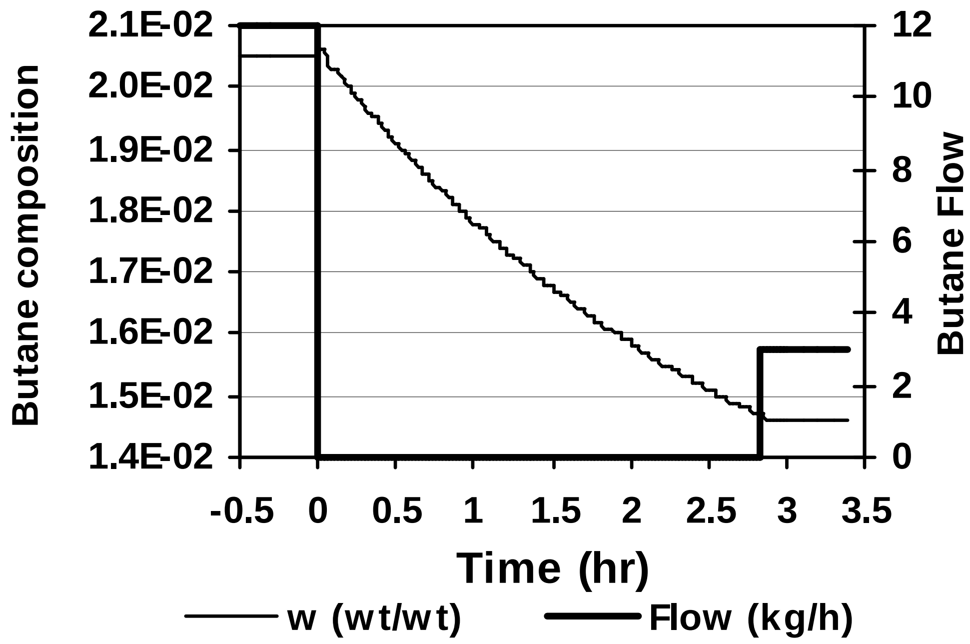


Low Density Polyethylene Plant
Detailed Reactor Model

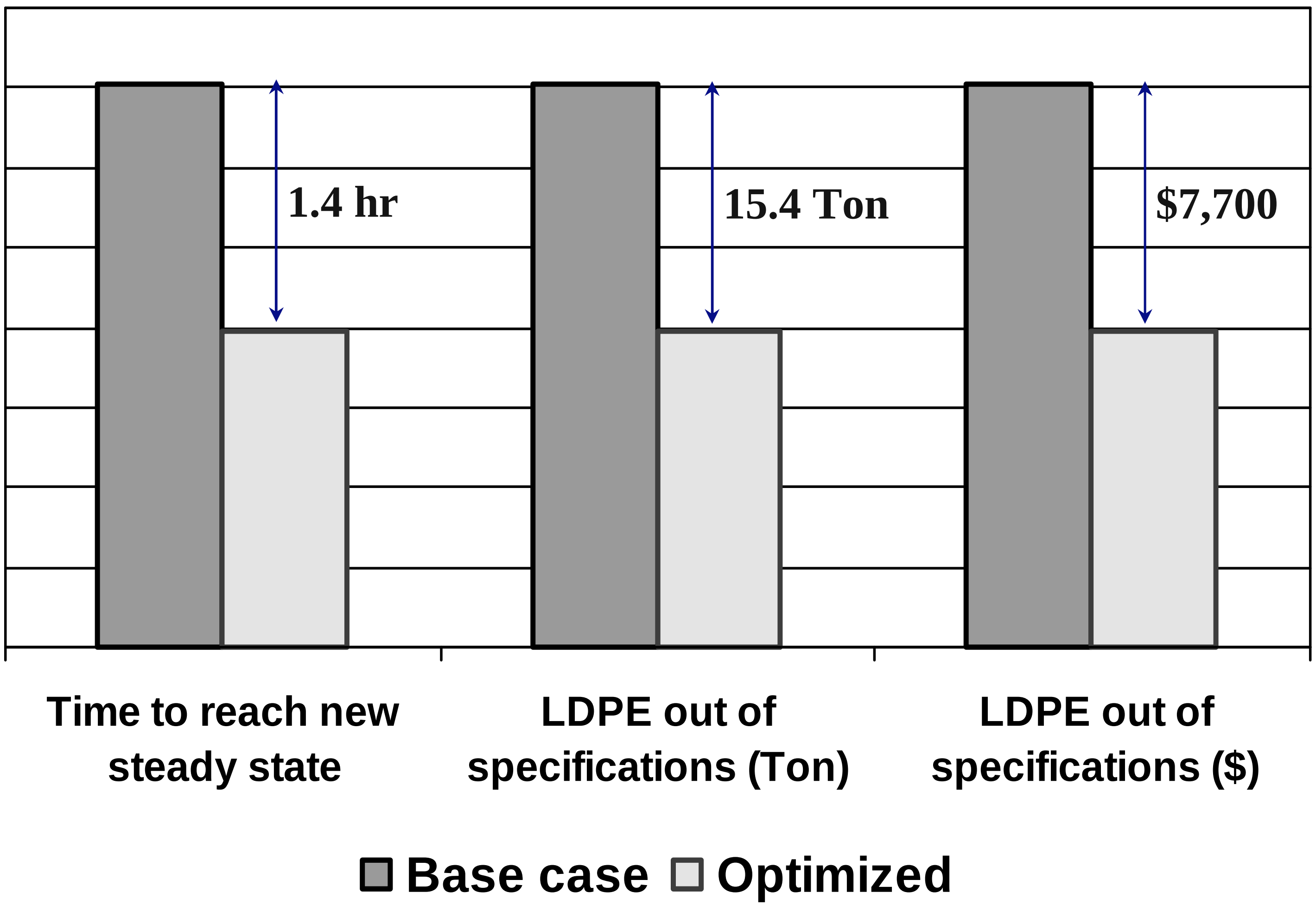
Increase Molecular Weight

- negligible change in optimal policy
- added moving finite elements for accurate states and controls (constant Hamiltonian)

- 532 DAEs
- 40 elements
- 3 collocation points
- 83,845 variables
- 3728.4 CPU s (P3)



Low Density Polyethylene Plant
Savings with optimal grade transition



What About Discrete Decisions in Dynamic Systems?

Differential Variational Inequalities (DVIs)

- Hybrid systems with variable structures
- Differential Nash Games
- Rigid Body Mechanics

Bilevel and Multilevel Optimization

- Economic Equilibrium Models
- Metabolic Models

Modeling interfacial and phase phenomena

- Capillary press. by different phases
- Disappearing equilibrium phases

MINLP Strategies

•Introduce binary decision variables

•Solve nonlinear optimization repeatedly for different instances of binaries

•Widely used in process design and logistics

Complementarity Constraints ($x\ y = 0;\ x, y \geq 0$)

•No discrete variables, single level nonlinear optimization problem

•Several ad hoc applications in RTO

•Leads to singular system of equations

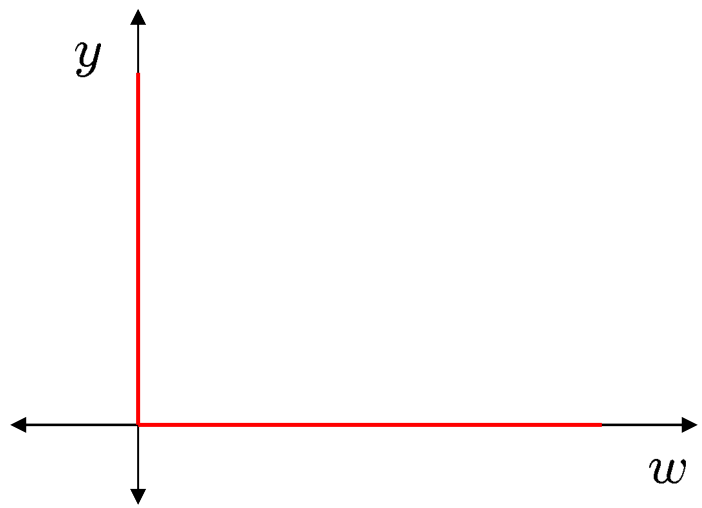
•Recent work in optimization community

MPCCs are not well-posed

$$\min_{x,w,y\in\mathbb{R}} \quad f(x,w,y)$$
$$\text{s.t.} \quad h(x,w,y) = 0$$
$$w, y \geq 0$$
$$wy = 0$$

There exist no (x,w,y) feasible to MPCC such that $w, y > 0$

- No strictly feasible points
- Gradients of constraints are linearly dependent
- Non-convex



Jacobian of constraints - singular at any feasible point

An Interior Point approach

MPCC

$$\begin{array}{ll} \min\limits_{x\in\mathbb{R}^n, w,y\in\mathbb{R}^m} & f(x,w,y) \\ \text{s.t.} & w,y \geq 0 \\ & w^{(i)}y^{(i)} = 0 \end{array}$$

Provide Interior $\Rightarrow$

NLP(t)

$$\begin{array}{ll} \min\limits_{x\in\mathbb{R}^n, w,y\in\mathbb{R}^m} & f(x,w,y) \\ \text{s.t.} & w,y \geq 0 \\ & w^{(i)}y^{(i)} \leq t \end{array}$$

Apply Interior Point approach

NLP(t,μ)

$$\begin{array}{ll} \min & f(x,w,y) - \mu \sum\limits_{i=1}^{m} \ln(w^{(i)}) - \mu \sum\limits_{i=1}^{m} \ln(y^{(i)}) \\ & -\mu \sum\limits_{i=1}^{m} \ln(s^{(i)}) \\ \text{s.t.} & w^{(i)}y^{(i)} + s^{(i)} = t \end{array}$$

$t \longrightarrow 0$ - recover complementarity

$\mu, t \longrightarrow 0$ - recover a solution of MPCC

IPOPT-C: NLP extended to MPCCs

Interface to AMPL modeling language

Numerical testing on 140 MPECs (MacMPEC)

Column and Tray Optimization

- Binary and 5-component feed
- Ideal thermodynamics

Start-up of distillation columns

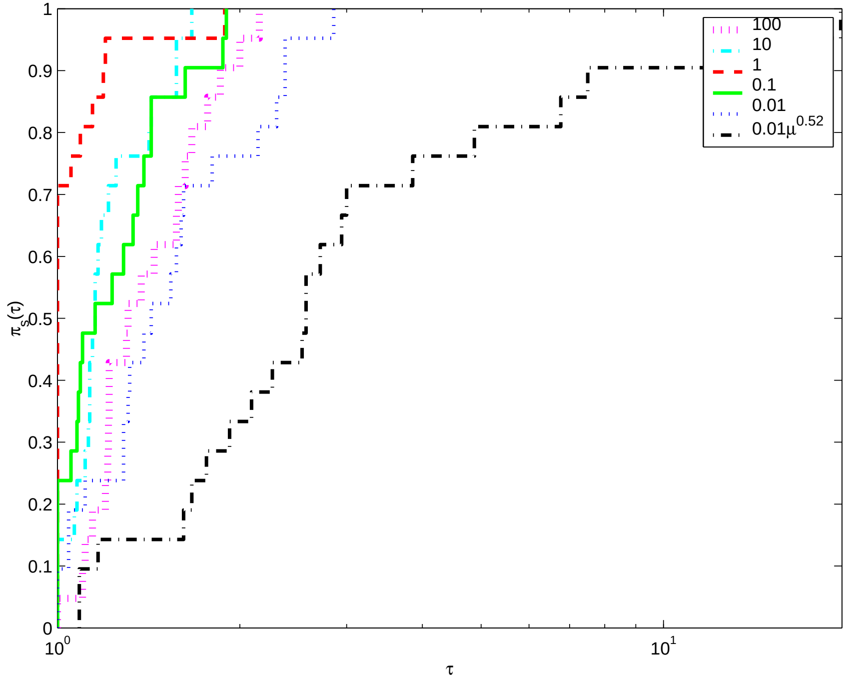
- Batch distillation
- Cryogenic column

Modeling Capillary Pressure in Oilfield Reservoirs

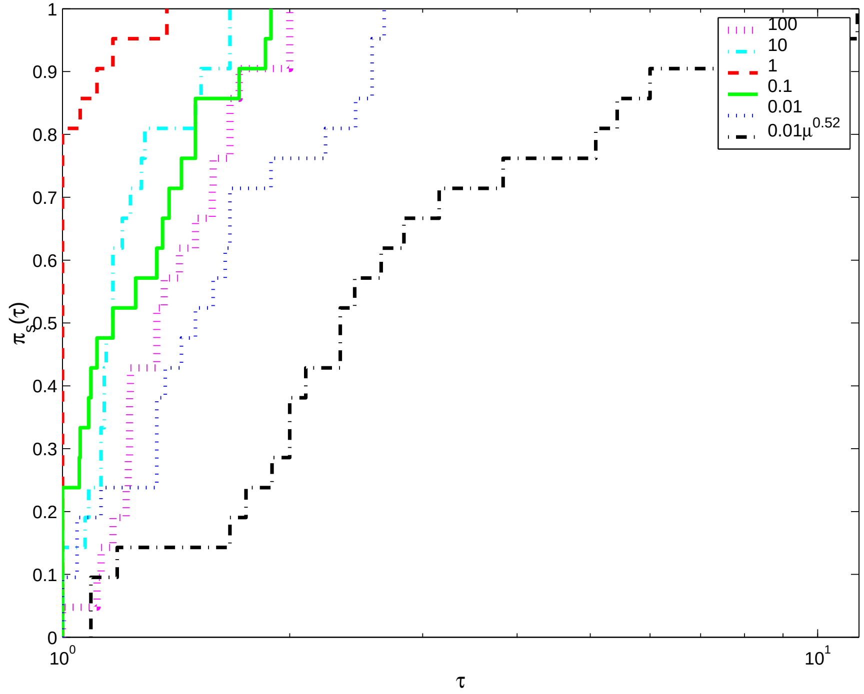
Data reconciliation & Parameter estimation (DRPE) in metabolic networks

IPOPT-C on MacMPEC problems (satisfying assumptions)

Function evaluations

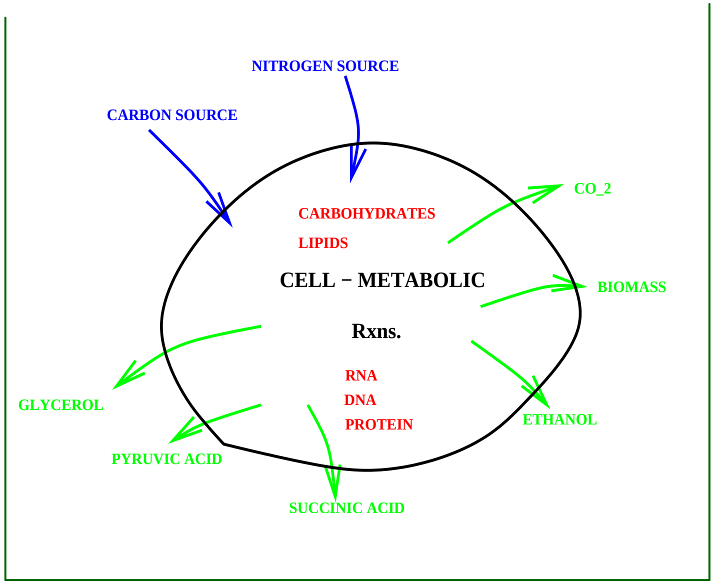


Iteration count



$\mu = 100t$	$\mu = 10t$	$\mu = t$
$\mu = 0.1t$	$\mu = 0.01t$	$\mu = 0.01t^{2.08}$

Yeast Fermentation for Wine-making



- Reactor is charged with substrates
- Cell metabolism
- Metabolic products accumulate
- Cell adaptation
  - depletion of substrates
  - increase in toxicity

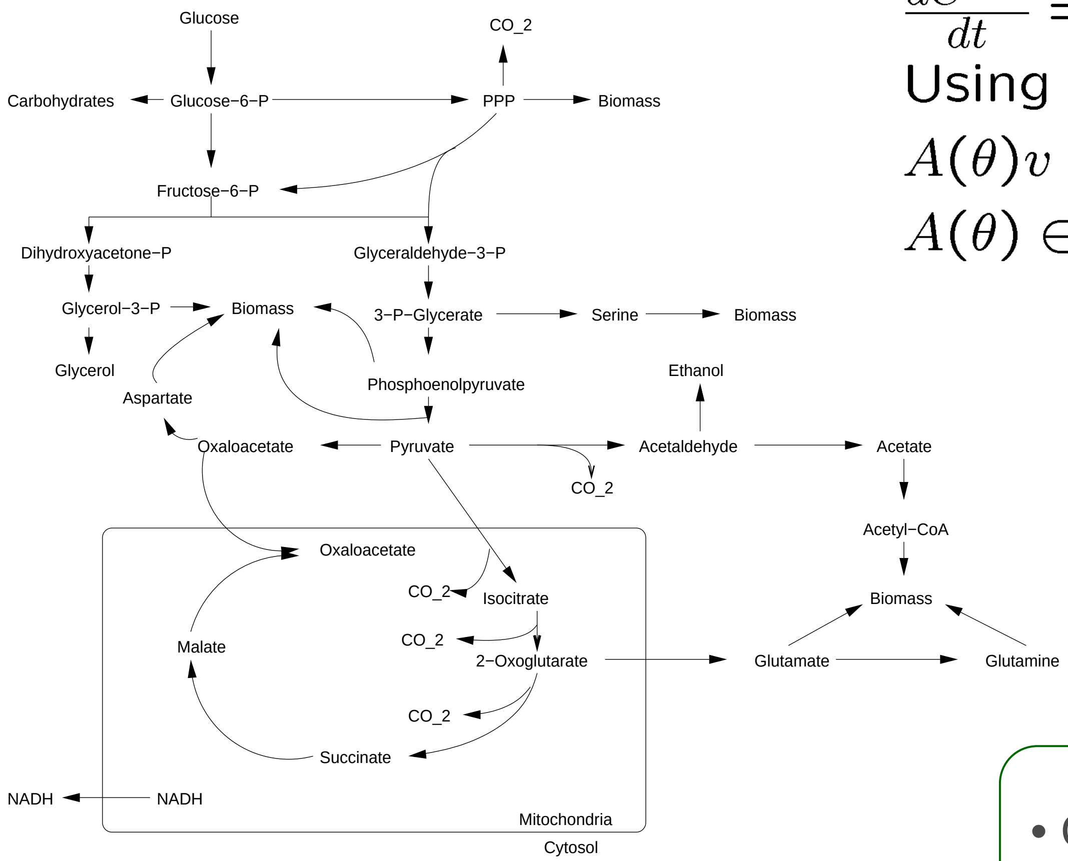
- Little understanding of fermentation problem fermentations
- Assume decomposition of time scales

- Metabolite accumulation in medium
- Cell metabolism
- Cell adaptation mechanisms

Enables online monitoring and control

Modeling approach of Sainz et al. (2003)

Cellular metabolism



Θ – Biomass parameters

$$\frac{dC^{\text{cell}}}{dt} = A(\theta)v - r$$

Using no intracellular accumulation

$$A(\theta)v = r,\ v \geq 0$$

$$A(\theta) \in \mathbb{R}^{m \times n}, v \in \mathbb{R}^n, r \in \mathbb{R}^m$$

v - reaction rates

r - metabolite rates

$r^{(i)} < 0$ - substrate

$r^{(i)} = 0$ - intracellular

$r^{(i)} > 0$ - product

- Given r, $m < n$ – underdetermined
- Measure concentration not r

Θ_{carb} Carb. + θ_{DNA} DNA + θ_{RNA} RNA + $\theta_{\text{Lip.}}$ Lipids + $\theta_{\text{Pro.}}$ Proteins → Biomass

Cellular metabolism

LP models cell metabolism

$$
\begin{aligned}
\text{min} \quad & d^T v \\
\text{s.t.} \quad & A(\theta)v = r \\
& v^L \le v \le v^U \\
& r^L \le r \le r^U
\end{aligned}
$$

Objective : biomass max. or maintenance

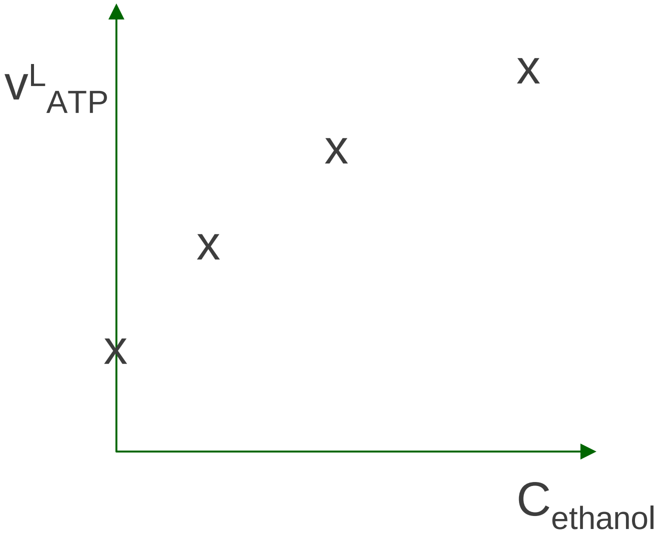
Solution provides

- intracellular reaction rates
- rate of substrate accumulation
- rate of metabolite production
- Bounds ?

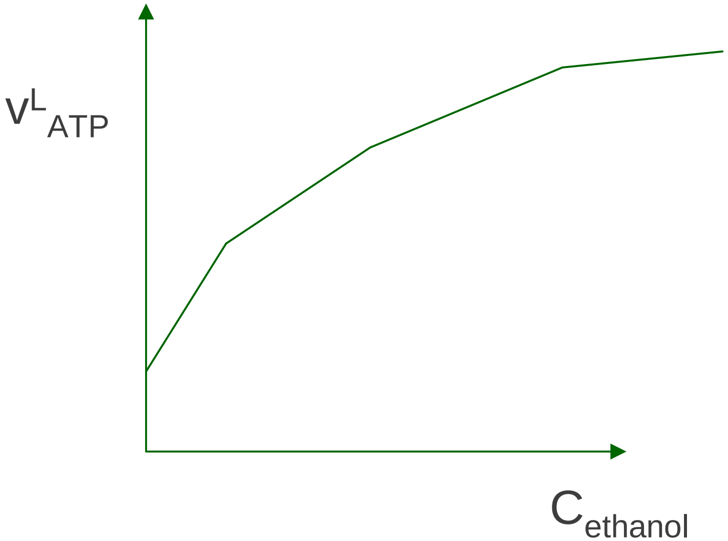
Given θ, constant bounds
$\Rightarrow$ No change in solution
Adaptation ?

Cellular adaptation

Response to single stimulus



→



$$
\begin{aligned}
\text{min} \quad & d^T v \\
\text{s.t.} \quad & A(\theta) v = r \\
& v^L(C) \leq v \leq v^U(C) \\
& r^L(C) \leq r \leq r^U(C)
\end{aligned}
$$

C - concn. of metabolites in medium

- Flux bound look-up tables
- Link extracellular concs. to cellular metabolism

Batch Fermentation Model Switching in Objectives

Depletion of nitrogen inhibits growth

Number of metabolic rates vanish

Results in degeneracy.

Metabolic Model Switching

$$C_{\text{ammonium}} > \epsilon$$

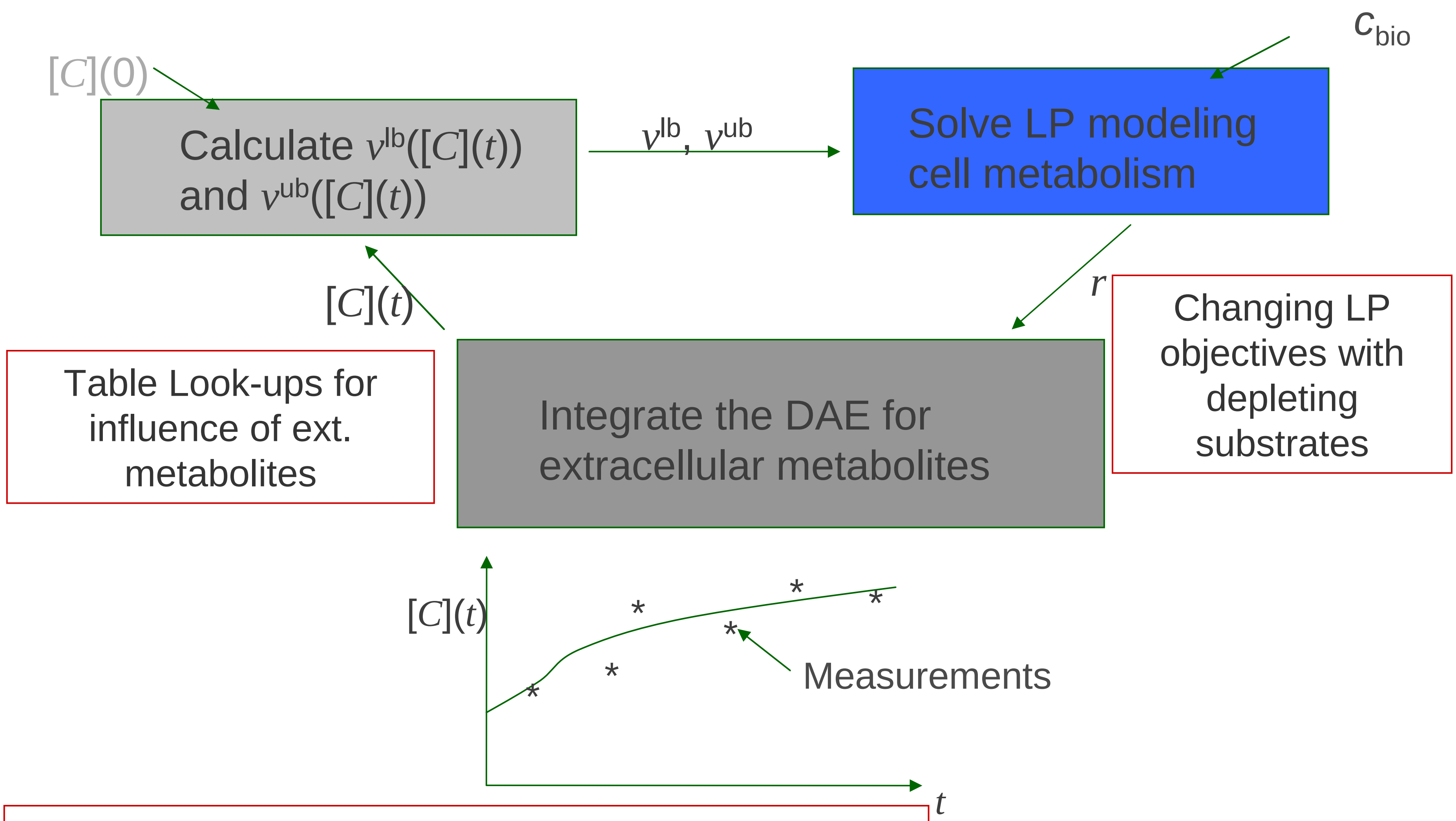
$$\begin{array}{ll} \text{min} & d_1^T v \rightarrow \text{Max. biomass} \\ \text{s.t.} & A_1(\theta) v = r \\ & v^L(C) \leq v \leq v^U(C) \\ & r^L(C) \leq r \leq r^U(C) \end{array}$$

$$C_{\text{ammonium}} \leq \epsilon$$

$$\begin{array}{ll} \text{min} & d_2^T v \rightarrow \text{Min. ATP} \\ \text{s.t.} & A_2(\theta) v = r \\ & v^L(C) \leq v \leq v^U(C) \\ & r^L(C) \leq r \leq r^U(C) \end{array}$$

Handled using complementarity constraints

Batch Fermentation : Combined Formulation



- Large-scale dynamic parameter estimation problem
- Many time-dependent complementarity constraints
- Solved as single large-scale nonlinear program

Batch Fermentation – Parameter estimation

Given $C^{\text{meas},(i)}$ for $i \in MEAS \subseteq EXMET$,
$t \in TMEAS_i \subseteq [0, T]$

$$\min_{\theta} \sum_{i \in MEAS} \sum_{t \in TMEAS_i} (C^{(i)}(t) - C^{\text{meas},(i)}(t))^2$$

$$\text{s.t.} \quad \text{LP}(\theta, v^L, v^U, r^L, r^U) \quad t \in [0, T]$$

$$\text{Flux bound defn.} \ v^L(C), v^U(C), r^L(C), r^U(C) \quad t \in [0, T]$$

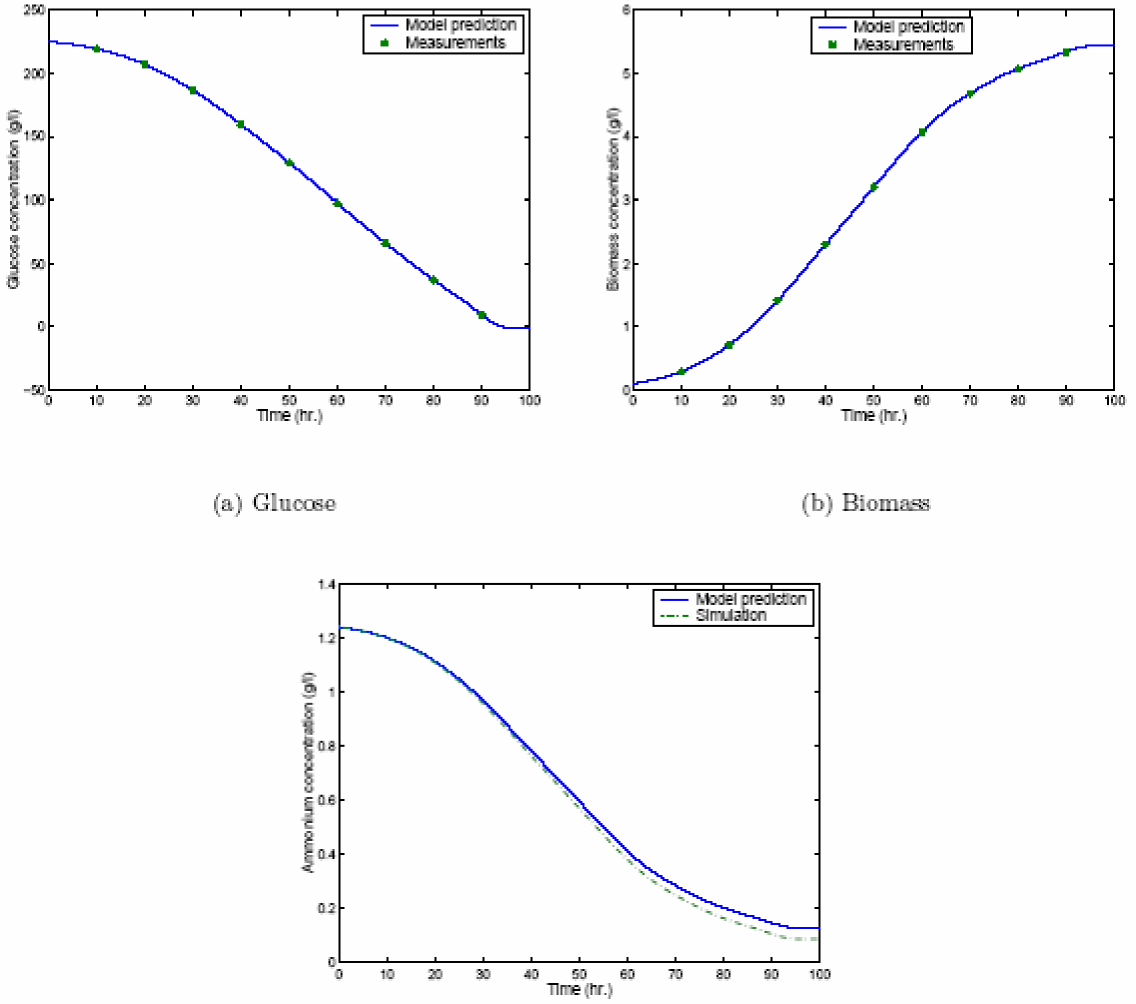
$$\frac{dC^{(i)}}{dt} = r^{(i)} C_{\text{biomass}} \quad t \in [0, T], i \in EXMET$$

LPs or VIs,
Flux bounds

$\longrightarrow$

Complementarity
Constraints

Batch Fermentation : Results with Simulated Data

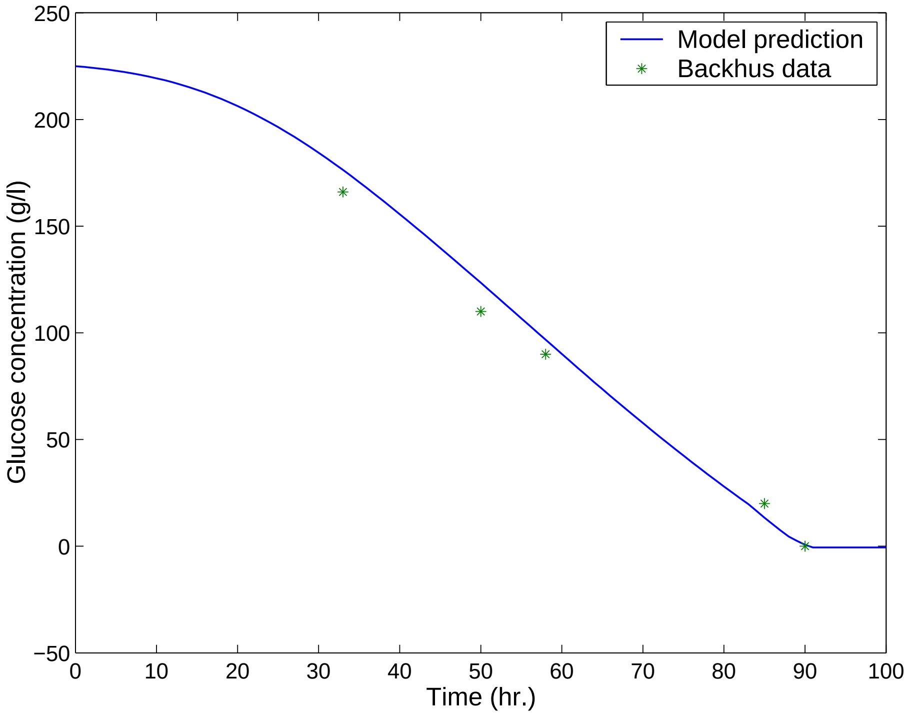


(a) Glucose

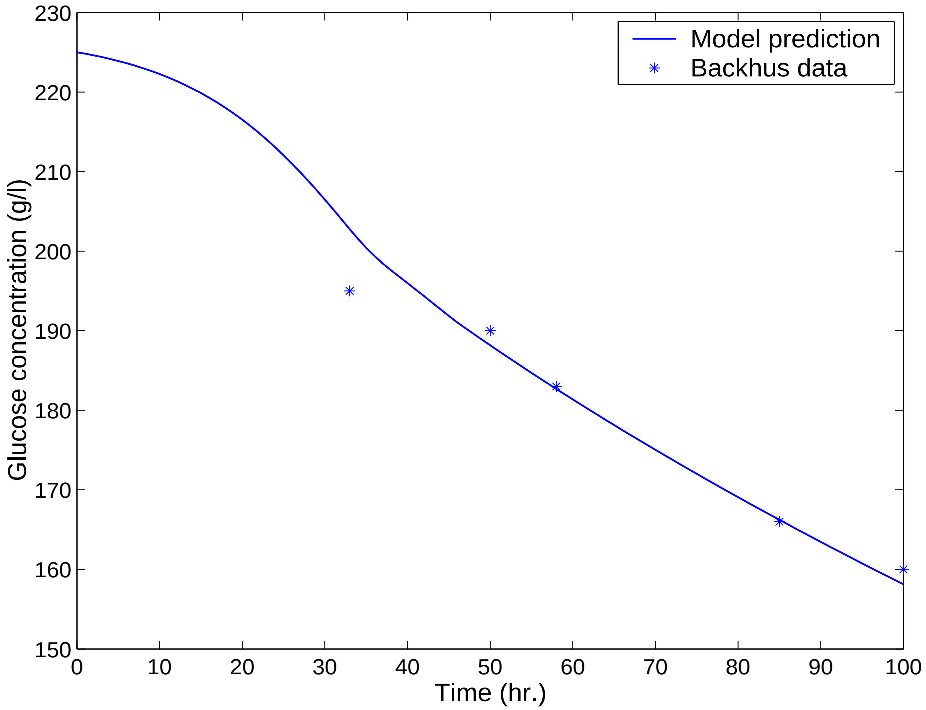
(b) Biomass

(c) Ammonium

Nitrogen rich



Nitrogen lean



Excellent fit to glucose experimental data

Model limitations lead to over-prediction of biomass data

Provides reasonably accurate model of wine fermentation

Batch Fermentation – Results
(Raghunathan, Perez, Agosin & B, 2004)

C(0)	Nitrogen-rich	Nitrogen-lean
Glucose	225	225
Biomass	0.1	0.1
Ammonium	1.24	0.165
Ethanol	0	0
CO_2	0	0

	Nitrogen-rich	Nitrogen-lean
# variables	33066	37328
# constraints	26192	29583
# complementarity	6870	7740
CPU time (sec.)	133	463

Conclusions

Goal: Nonlinear programming formulations and algorithms that expand the scope of model building, validation and optimization applications

Interior Point NLP (IPOPT)

Novel line search approach

Comprehensive open source code with extensive testing

Guaranteed convergence properties

Many dynamic optimization applications

Solved NLPs with up to 2 million variables, 5000 degrees of freedom

Math Programs with Complementarity Constraints (MPCCs)

Handle nested (bilevel) optimization problems

Deal with (some) discrete decisions

Wealth of discrete/continuous applications

Specialized NLP solver developed: IPOPT-C

Local solutions only, but very fast convergence

Acknowledgements

Coworkers

- Juan Arrieta
- Arturo Cervantes
- Arvind Raghunathan
- Andreas Wächter

Funding Sources

- CONACYT Fellowship
- UNAM Fellowship
- DARPA/Honeywell
- National Science Foundation
- ExxonMobil