Steady-state constrained optimisation for input/output large-scale systems using model reduction technology

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Outline

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- The Reduced Hessian method
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Motivation

- The construction of a steady-state optimisation framework
  - gradient-based (deterministic)
  - constrained
  - for large-scale systems
  - including a few degrees of freedom compared with dependent variables
    - Typical situation in engineering design problems
  - using steady-state, iterative simulators
    - computationally efficient for large-scale non-linear problems
- Wraps around existing (e.g. commercial/black-box) simulators
- Computationally efficient
  - Based on model reduction technology
- Extend the optimisation schemes designed for dynamic simulators*

*Luna-Ortiz, E. and C. Theodoropoulos (2005) Multiscale Modeling & Simulation 4(2): 691-708.

*C. Theodoropoulos and Luna-Ortiz (2006) in Model reduction and coarse-graining approaches for multiscale phenomena, p.535-560

The optimisation problem

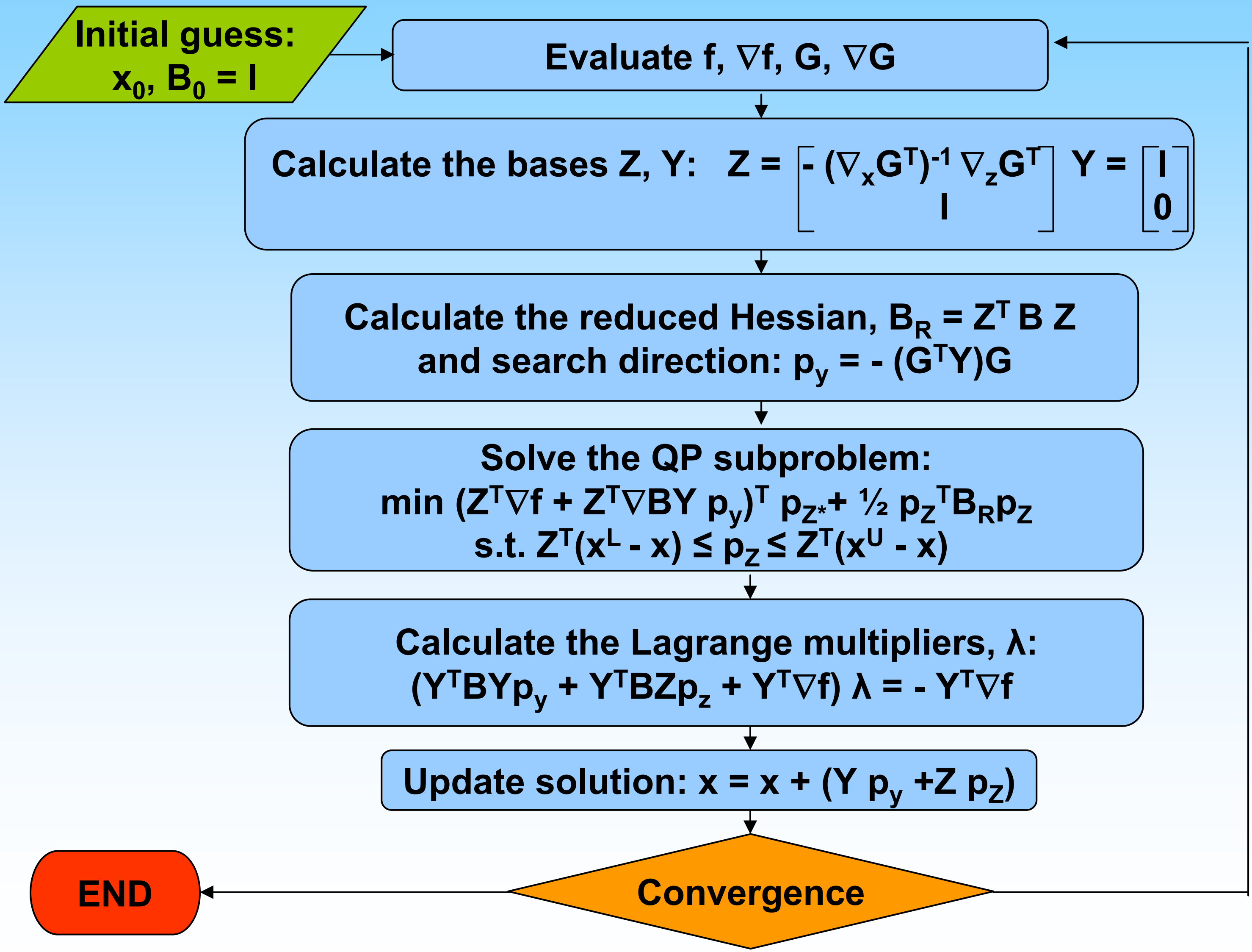
The algorithm presented here:

- deals with the optimisation problem:

$$\min f(x)$$
$$\text{s.t. } G(x) = 0,$$
$$H(x) \leq 0 \ \text{ and}$$
$$x^L \leq x \leq x^U$$

- where x: $x^T = [u^T \ z^T]$, is the joint vector of:
  - the dependent (u) and
  - the independent (z) variables:
- An input/output simulator is used for the solution of G(x) = 0
  - A formula for the calculation of H(x) need not be explicitly provided as well

The reduced Hessian method



This method:

- decomposes the search space in two subspaces, with bases Z & Y
- Z spans the tangent space of $(\nabla_x G)^T$
- It employs the solution of a QP subproblem in every iteration
- The QP is based on a reduced Hessian, of size equal to the number of degrees of freedom
- If steady states are calculated in every step, py = 0

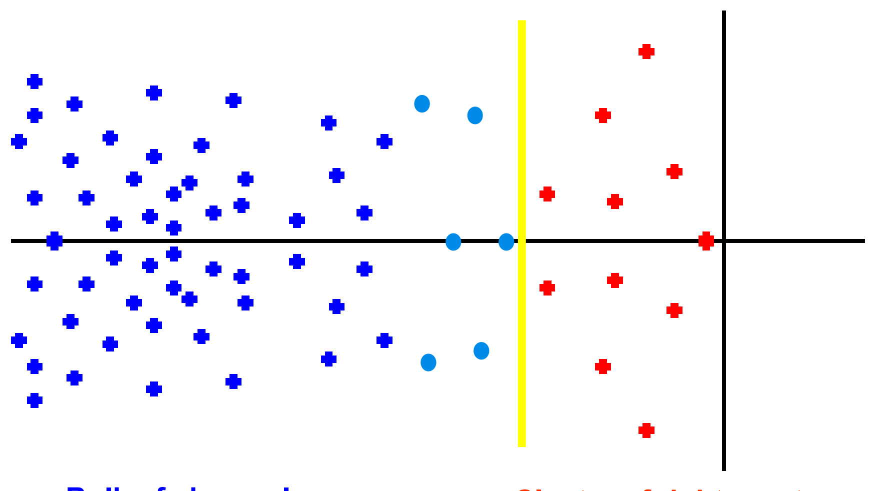
Problems

- Expensive for large problems
- Based on handling of large matrices
- Requires inverting the Jacobian in each step

*e.g.: Biegler, et al. (1995). Siam Journal on Optimization 5(2): 314-347

Model Reduction Technology

- The separation of scales is exploited for model reduction*
- Nominally, two clusters of eigenvalues in the eigenspectrum
  - There is a gap in between
  - The rightmost eigenvalues are the domimant ones
- We can work merely on the low-dimensional dominant subspace
  - Good approximation of the system



- Jacobians (H) and Hessians (B_R) involved in this formulation
  - low-dimensional
  - projections of the original ones onto the dominant subspace (P)
  - this subspace can be identified using subspace iterations

*Meerbergen, K., et al,Bit, 1994. 34(3): p. 409-423; Shroff, G.M. and H.B. Keller, Siam Journal on Numerical Analysis, 1993. 30(4): p. 1099-1120.

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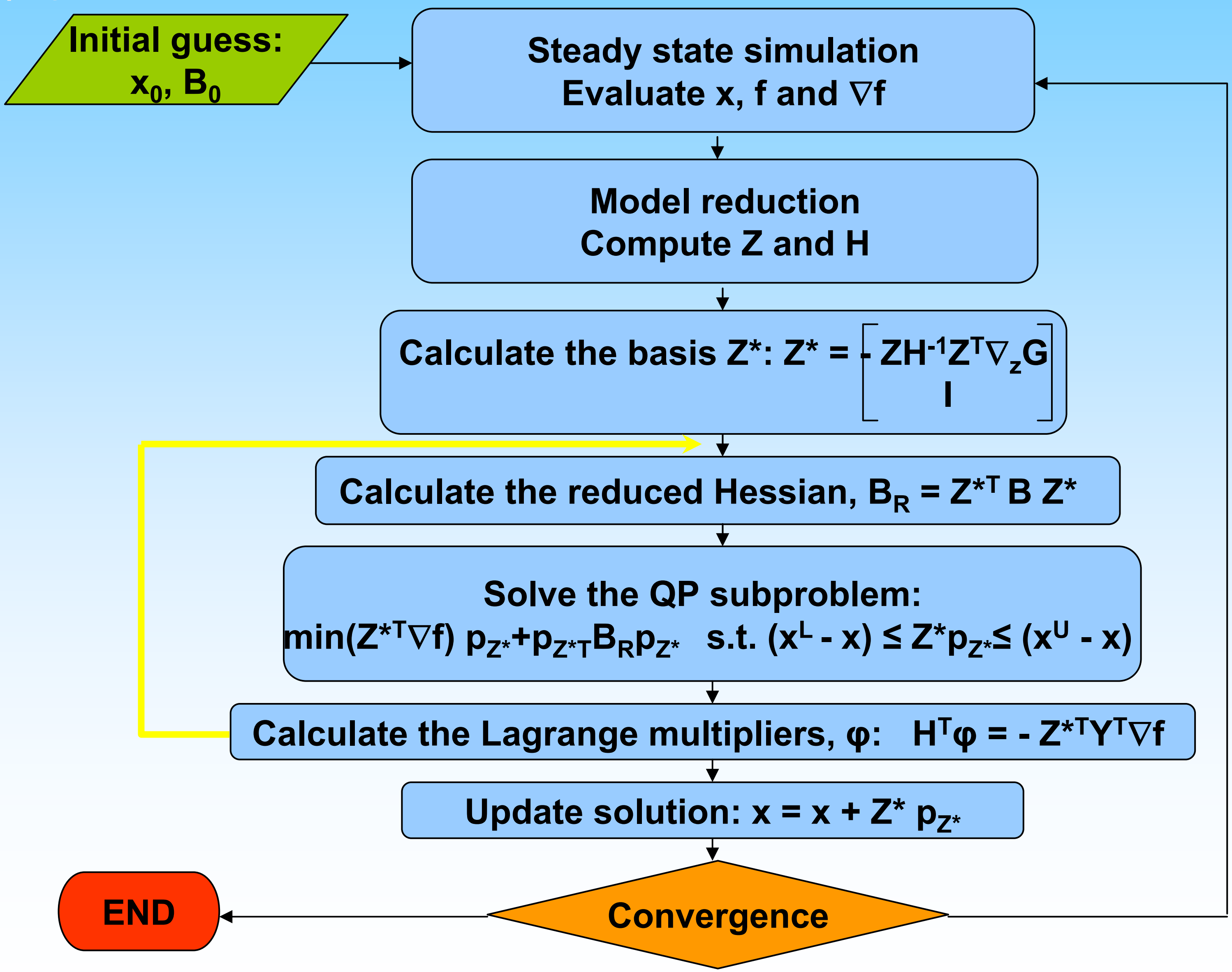
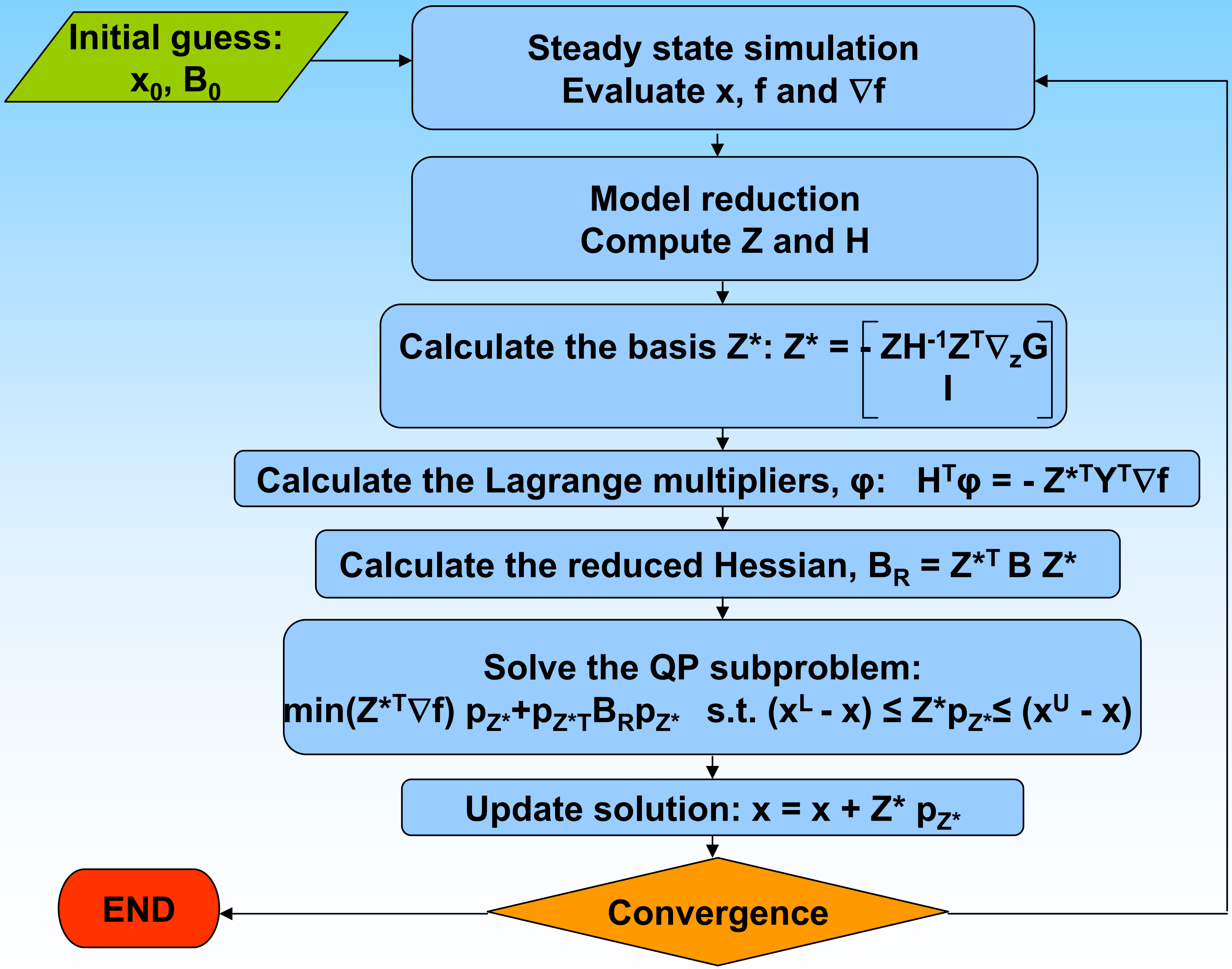
The proposed algorithm



The algorithm presented:

- Is model reduction-based
- Employs a 2-step projection
  - 1. onto the dominant system subspace
  - 2. onto the subspace of the degrees of freedom
- Only low-dimensional Jacobians (H) and Hessians (B_R) are used
- Those are calculated through numerical perturbations
- A QP subproblem is solved in every iteration, using projection of f

An improved version



The reordering:

- Implemented to reduce computational cost
- Lagrange multipliers are calculated before updating B_R
- No need to update the basis after the QP step
- Subspace iterations are used only once per iteration
- Is based on assumption:
  - the basis for the dominant subspace after QP step good approximation of the basis for the feasible point of the next iteration
- This incurs loss of accuracy
- For the first iterations we use the reordered version of the algorithm
- Near the optimum point we revert to the standard algorithm
- Computational gain: ~10-20%

Projections

First Projection:

- P the low-dimensional dominant subspace
  - identified adaptively through subspace iterations
  - Let Z an low-dimensional orthonormal basis for this subspace
  - Z is extended to include the subspace of the independent variables:

$$Z_{ext} = \begin{bmatrix} Z & 0 \\ 0 & I \end{bmatrix}$$

- So the 1st projection is onto the dominant subspace and is orthogonal

Second Projection:

- Onto the subspace of degrees of freedom
  - Also low-dimensional but non-orthogonal
- The corresponding basis Z_r now only based on H
  - $Z_r = \begin{bmatrix} -H^{-1} Z^T \nabla_z G \\ I \end{bmatrix}$

The 2-step projection

- The basis for the overall projection is $Z^* = Z_{ext} Z_r =$

$$\begin{bmatrix} Z & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} -H^{-1} Z^T \nabla_z G \\ I \end{bmatrix} = \begin{bmatrix} -Z H^{-1} Z^T \nabla_z G \\ I \end{bmatrix}$$

  - where H is the projection of the Jacobian
    - onto the dominant subspace **P**: $H = Z^T \nabla_u G^T Z$
- So reduced Hessian is now computed:
  - $B_R = Z^{*T} B Z^* = Z_r^T (Z_{ext}^T B Z_{ext}) Z_r$
- Computation of the low-dimensional Hessian
  - based on numerical directional perturbations to the direction of Z
- Lagrange multipliers are also needed to calculate B
- In reduced Hessian calculated by: $\lambda = -(\nabla_u G)^{-1} \nabla_u f$, $\lambda \in \Re^N$
  - where N is the number of dependent variables
- Here projection of λ onto **P**: $\varphi = Z\lambda = -(H^T)^{-1} Z^T \nabla_u f$ $\varphi \in \Re^m$
  - where m is the size of the basis Z

Handling of inequality constraints

- The inequality constraints are aggregated using a KS function*
- For a set of inequality constraints, $h_j(x) \leq 0$, the KS function is:

$$KS(h_j) = \frac{1}{\rho}\ln\left[\sum_{j=1}^{J}\exp\left(\rho h_j\right)\right] \quad \text{or} \quad KS(h_j) = M + \frac{1}{\rho}\ln\left[\sum_{j=1}^{J}\exp\left(\rho(h_j - M)\right)\right], \quad M \approx \max(h_j)$$

  - The 2 forms are equivalent, the second achieving better numerical robustness
  - 2 important properties of KS: $KS(x,\rho) \geq \max_j\left(h_j(x)\right), \rho > 0$ and $\lim_{\rho\to\infty} KS(x,\rho) = \max_j\left(h_j(x)\right)$
- So the optimisation problem becomes:

$$\min f(x) \quad \text{s.t. } h_j(x) \leq 0 \quad \Rightarrow \quad \min f(x) \quad \text{s.t. } KS(x,\rho) \leq 0$$

- The objective function can be modified to include the KS function**
  - Eliminating all inequality constrains
- In the proposed optimisation scheme
  - The inequality constraints are aggregated following the KS approach
  - The projection of the KS function is added to the objective function
  - Hence the extra computational cost is minimal

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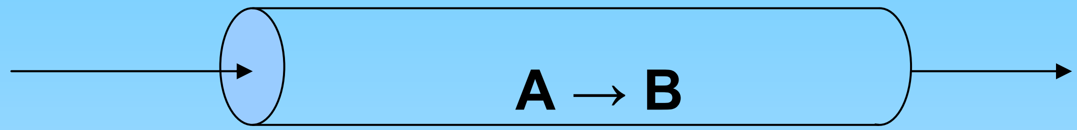
* C.G.Raspanti, et al, Computers and Chemical Engineering 24 (2000) 2193-2209

** G.C.Itle et al, Computers and Chemical Engineering 28 (2004) 291-302.

Case study I: The tubular reactor



- ***The model of the reactor consists of two PDEs*[*]*. At s.s.:***

$$\frac{1}{Pe_1}\frac{\partial^2 x_1}{\partial y^2} - \frac{\partial x_1}{\partial y} + Da(1-x_1)\exp\left(\frac{x_2}{1+x_2/\gamma}\right) = 0$$

$$\frac{1}{LePe_2}\frac{\partial^2 x_2}{\partial y^2} - \frac{1}{Le}\frac{\partial x_2}{\partial y} - \frac{\beta}{Le}x_2 + \frac{C}{Le}Da(1-x_1)\exp\left(\frac{x_2}{1+x_2/\gamma}\right) + \frac{\beta x_{2w}}{Le} = 0$$

  - where x_1: dimensionless reactant concentration and
  - x_2: dimensionless temperature,

- ***Boundary conditions:***

$$\frac{\partial x_1}{\partial y} - Pe_1 x_1 = 0, \quad \frac{\partial x_2}{\partial y} - Pe_2 x_2 = 0 \quad \text{at} \quad y = 0 \quad \text{and} \quad \frac{\partial x_1}{\partial y} = 0, \quad \frac{\partial x_2}{\partial y} = 0 \quad \text{at} \quad y = 1$$

- ***Parameter values***

  - $Le = 1.0$, $Pe_1 = Pe_2 = 5.0$, $\gamma = 20.0$, $\beta = 1.50$, $C = 12.0$, $Da = 1.0$

- Discretized in 250 nodes using Finite Differences producing 500 unknowns

[*]Jensen, K. F. and W. H. Ray (1982). Chemical Engineering Science 37(2): 199-222

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Optimisation with 1 degree of freedom

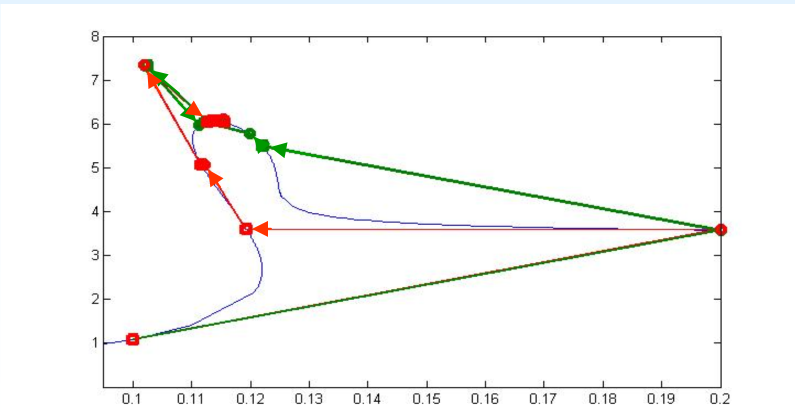
Problem statement

$$\max_{Da} x_2\big|_{exit} \quad s.t.\ F_1 = 0,\ F_2 = 0,$$
$$0 \le x_1\big|_k \le 1,\ 0 \le x_2\big|_k \le 1,\ k \in \Omega$$

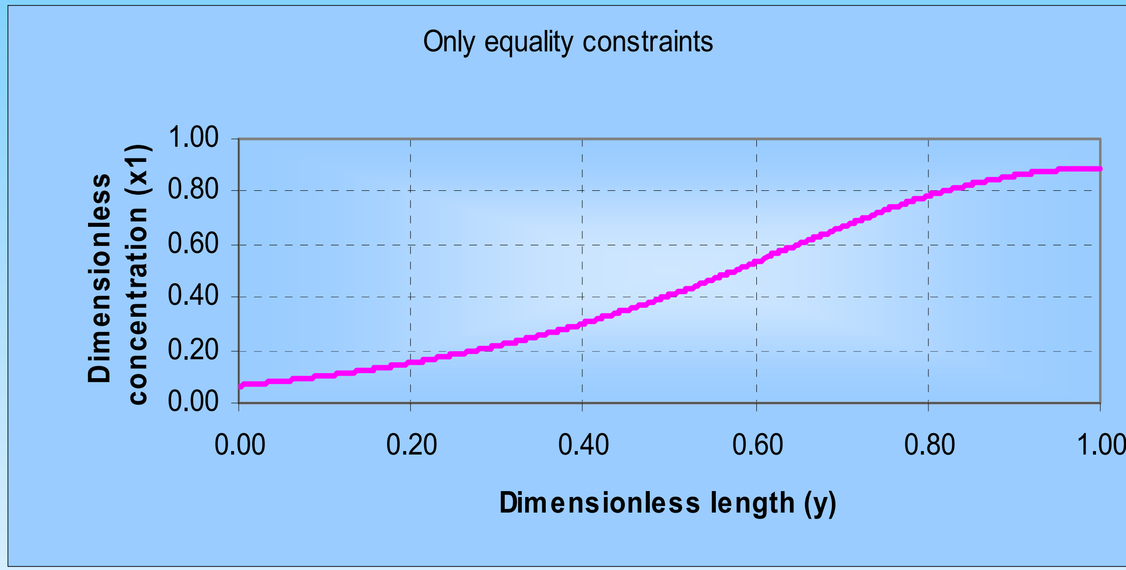
- Dominant subspace size: m=10

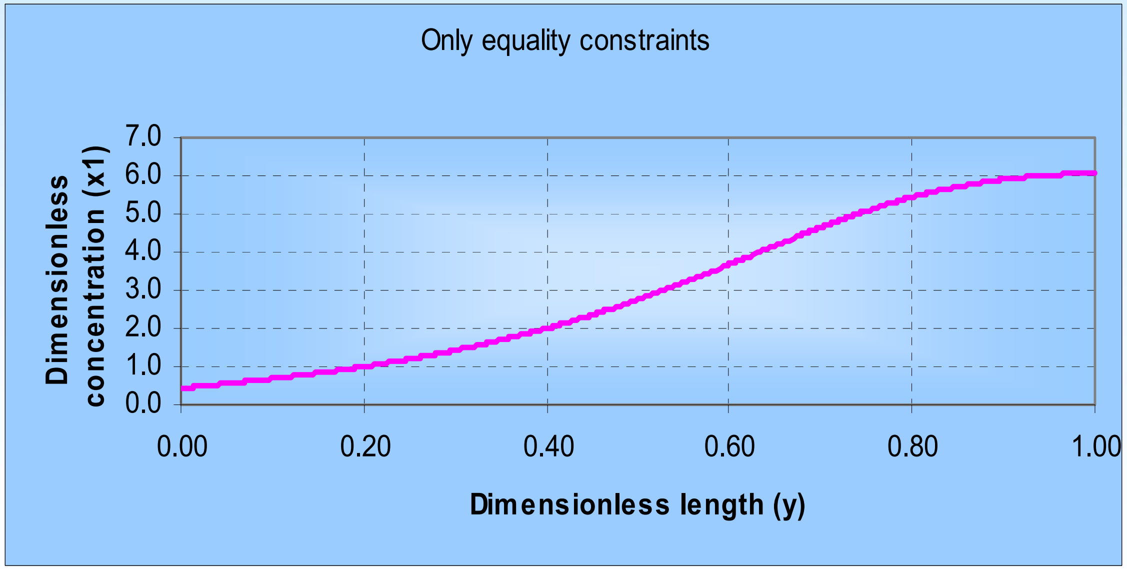
Results

- Convergence in 9 iterations
- Optimal Da = 0.1139
- Optimal dimensionless T = 6.055



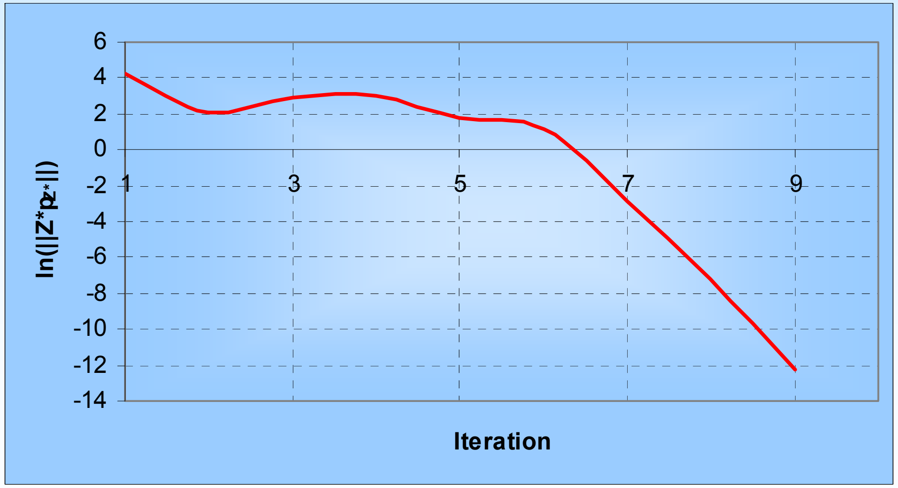
Optimisation path: ○: Newton steps; □: QP steps





Convergence data

Iter	x_{w1}	f	$\left\|Z^{*T}\nabla f\right\|$	||Z*pZ*||
1	2.001723	-0.99861	2.999592	1.70E-02
2	2.345387	-0.99937	4.136745	3.901032
3	2.556146	-0.99888	4.122835	1.068498
4	2.614274	-0.99871	4.136222	0.871199
5	2.528722	-0.9988	4.146356	0.344318
6	2.507706	-0.99884	4.156351	0.264178
7	2.483171	-0.99887	4.156247	1.46E-02
8	2.482629	-0.99887	4.156174	1.52E-04
9	2.482617	-0.99887	4.156174	9.93E-06



Convergence curves

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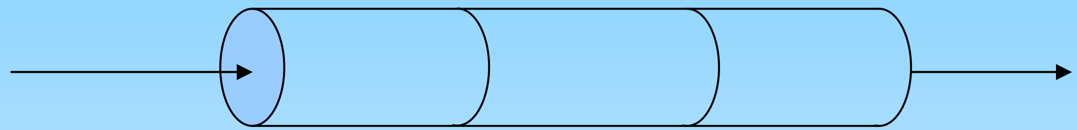
Reactor with 3 degrees of freedom

Tubular reactor with 3 cooling zones



- In this case the x_{2w} is given by:

$$x_{2_w}(y) = \sum_{j=1}^{3} [H(y - y_{j-1}) - H(y - y_j)] x_{2_w j} \qquad y_1 = 1/3, \quad y_2 = 2/3, \quad y_3 = 1$$

- the 3 wall temperatures (x_{2w}) are the independent variables

Problem Formulation

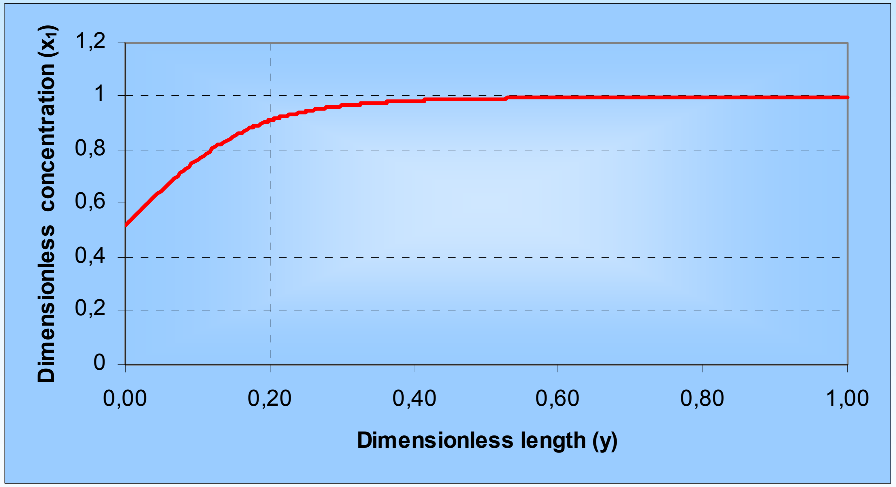
$$\begin{aligned} &\max_{x_{2wj}} x_1\big|_{exit} \\ &\text{s.t. } F_1 = 0, F_2 = 0, \\ &\quad 0 \le x_1\big|_k \le 1,\ 0 \le x_2\big|_k \le 1,\ k \in \Omega \end{aligned}$$

Numerical Details

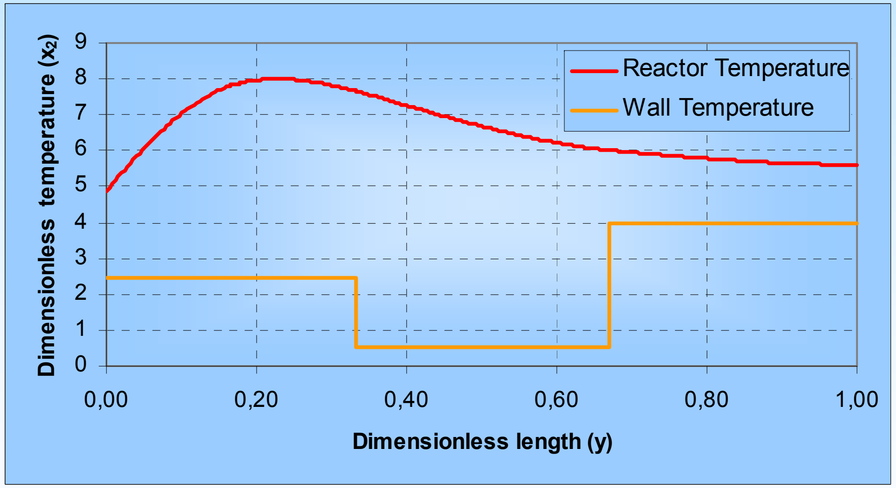
- Discretization using Finite Differences over a mesh of 250 nodes
  - 500 dependent variables (dimensionless concentrations and temperatures)
  - 3 independent ones (dimensionless temperatures of the cooling zones)

Results

- Size of the dominant subspace: m=10
- Convergence in 10 iterations
- Optimal values found:
  - $x_{2w,1} = 2.483$, $x_{2w,2} = 0.5254$, $x_{2w,3} = 4.000$.
  - Optimal $x_1|_{exit} = 0.99868$

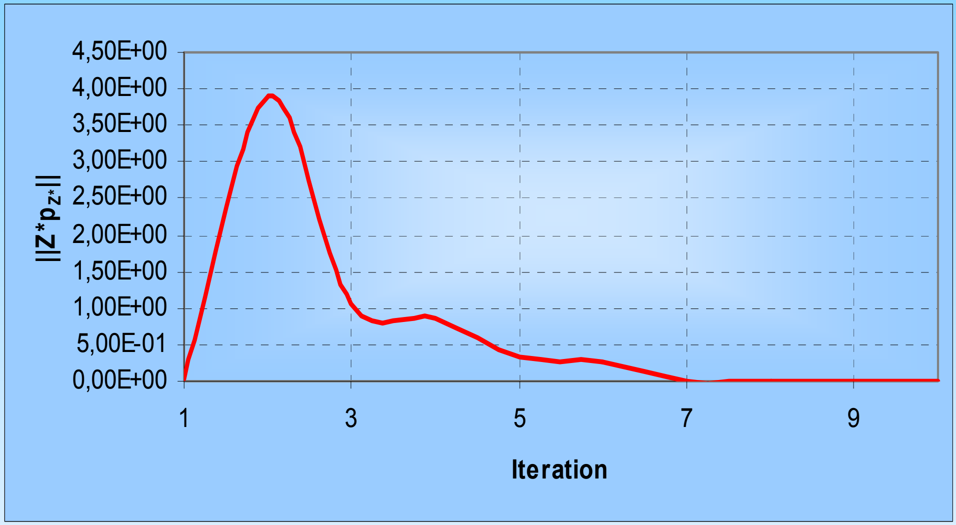


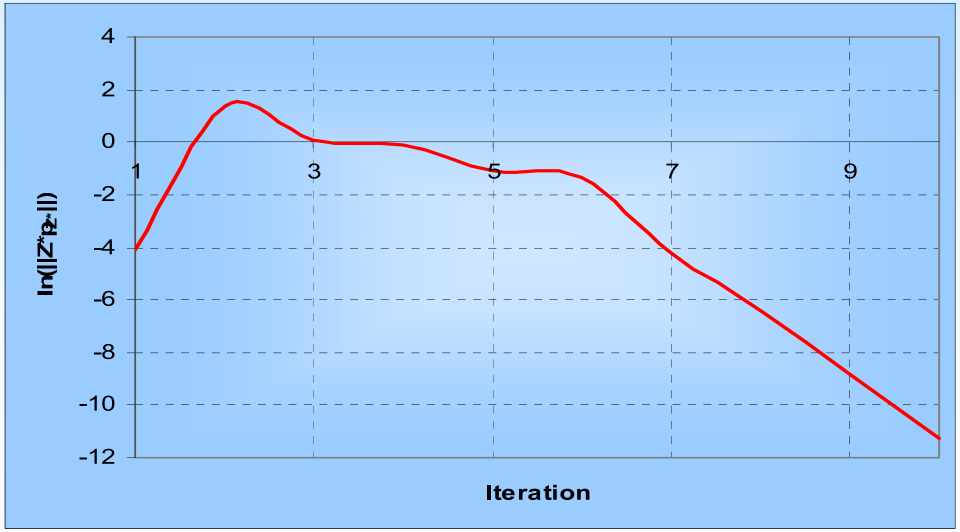
Dimensionless concentration profile for the optimum x_{2w}



Dimensionless temperature profile for the optimum x_{2w}

Convergence data





Iter	x_{w1}	x_{w2}	x_{w3}	f	$\|Z^{*T}\nabla f\|$	$\|\|Z^*pZ^*\|\|$
1	2.001723	1.999998	2.000082	-0.99861	2.999592	1.70E-02
2	2.345387	0.337519	4.000000	-0.99937	4.136745	3.901032
3	2.556146	0.00000	4.000000	-0.99888	4.122835	1.068498
4	2.614274	0.333037	4.000000	-0.99871	4.136222	0.871199
5	2.528722	0.441204	4.000000	-0.9988	4.146356	0.344318
6	2.507706	0.526858	4.000000	-0.99884	4.156351	0.264178
7	2.483171	0.525977	4.000000	-0.99887	4.156247	1.46E-02
8	2.48249	0.525341	4.000000	-0.99887	4.156166	1.59E-03
9	2.482629	0.525402	4.000000	-0.99887	4.156174	1.52E-04
10	2.482617	0.525397	4.000000	-0.99887	4.156174	9.93E-06

Optimisation including inequality constraints

Problem Statement (1DOF)

$$\max_{Da} x_2\big|_{exit} \quad s.t.\ F_1 = 0,\ F_2 = 0,$$

$$0 \le x_1\big|_k \le 1,\ 0 \le x_2\big|_k \le 1,\ k \in \Omega,$$

$$x_1^2\big|_k \le 4,\ k = \{125, \ldots, 130\}$$

Problem Statement (3DOFs)

$$\max_{x_{2wj}} x_1\big|_{exit} \quad s.t.\ F_1 = 0, F_2 = 0,$$

$$0 \le x_1\big|_k \le 1,\ 0 \le x_2\big|_k \le 8,\ k \in \Omega$$

$$\left(x_2\big|_k + x_2\big|_{k+1}\right)^2 \le 160,\ k = \{125, 127, 129\}$$

- Dominant subspace size: m=10 for both cases

Implementation

- The inequality constraints were treated using the KS approach.
- Scaled variables are defined: $\tilde{x}_1 = x_1 / \mu_1,\quad \tilde{x}_2 = x_2 / \mu_2 \quad with \quad \mu_1 \approx \max(x_1) \quad and \quad \mu_2 \approx \max(x_2)$
- A vector function for the nonlinear inequality constraints is defined:

$$h_i = \left(\tilde{x}_2\big|_k + \tilde{x}_2\big|_{k+1}\right)^2 - 40/\mu_2^{\,2},\ k = i + 124$$

- The KS function can now be computed:

$$KS(h_j) = M + \frac{1}{\rho}\ln\left[\sum_{j=1}^{J}\exp\left(\rho(h_j - M)\right)\right], \quad M \approx \max(h_j)$$

- The equivalent optimisation problem solved, is:

$$\max_{x_{2wj}} \left(\tilde{x}_1\big|_{exit} + KS(h_j)\right) \quad s.t.\ F_1 = 0,\ F_2 = 0,$$

$$0 \le x_1\big|_k \le 1,\ 0 \le x_2\big|_k \le 8,\ k \in \Omega$$

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Results for 1 dof case study

Objective

$$\max_{Da} x_2\big|_{exit}$$

$$s.t.\ F_1 = 0,\ F_2 = 0,$$

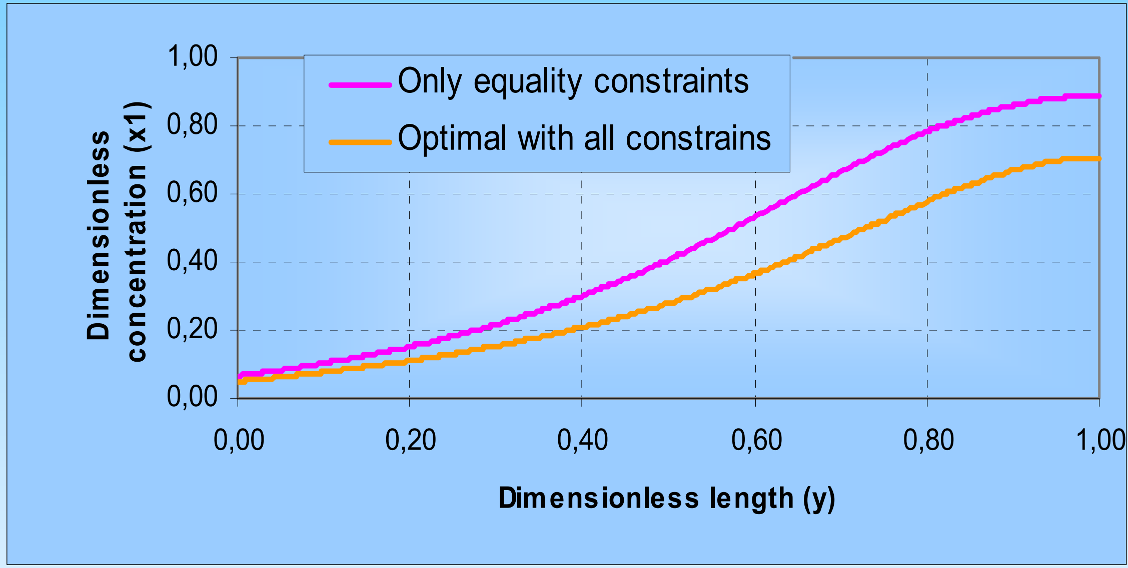
$$0 \le x_1\big|_k \le 1,\ 0 \le x_2\big|_k \le 1,\ k \in \Omega,$$

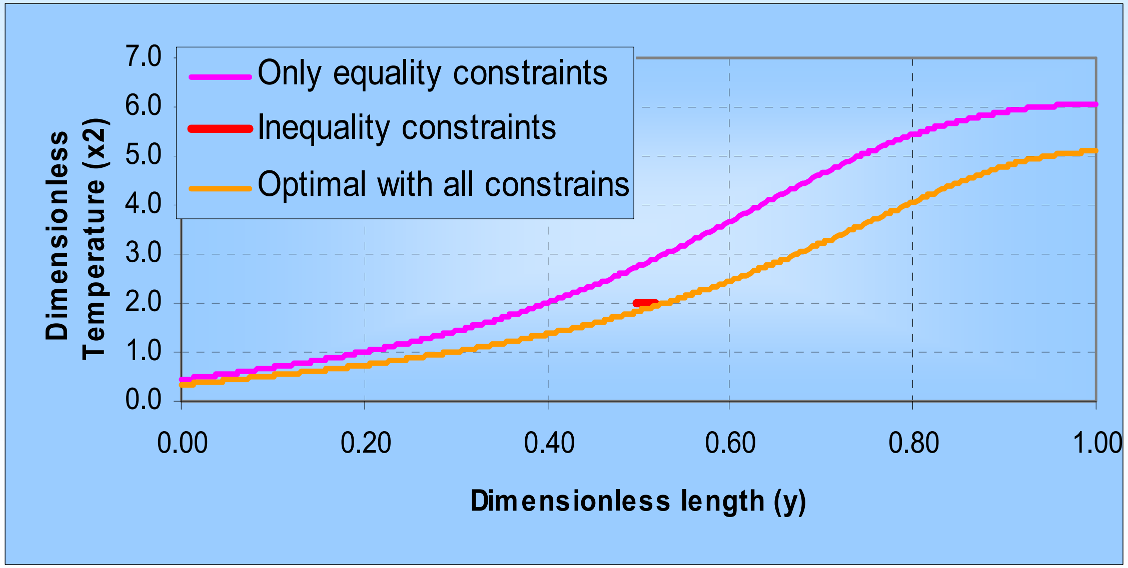
$$x_1^2\big|_k \le 4,\ k \in J = \{125,\ldots,130\}$$

- Dominant subspace size: m=10
- The inequality constraints were treated using the KS approach (Case B).

Results

- Convergence in 9 iterations
    - 12 if inequality constraints are considered
- The constraints are active and met
- Optimal Da found:
    - Case A: 0.1139 Case B: 0.1114
- Optimal dimensionless temperatures:
    - Case A: 6.055 Case B: 5.092





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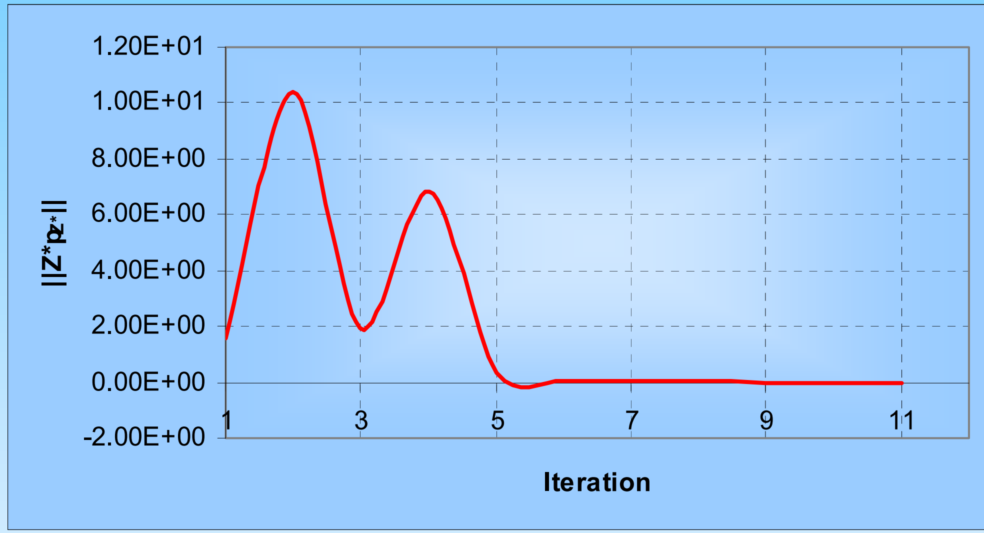
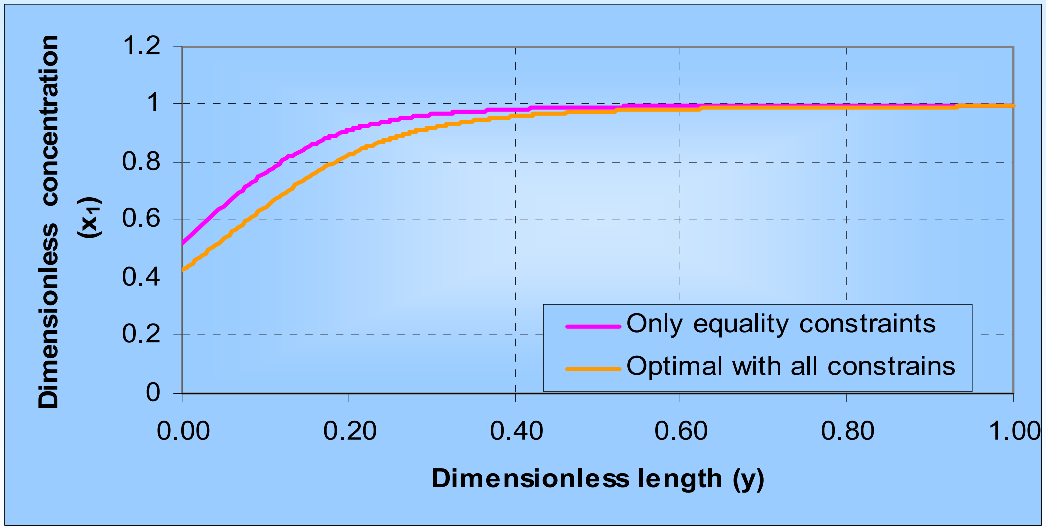
Results for 3 dof case study

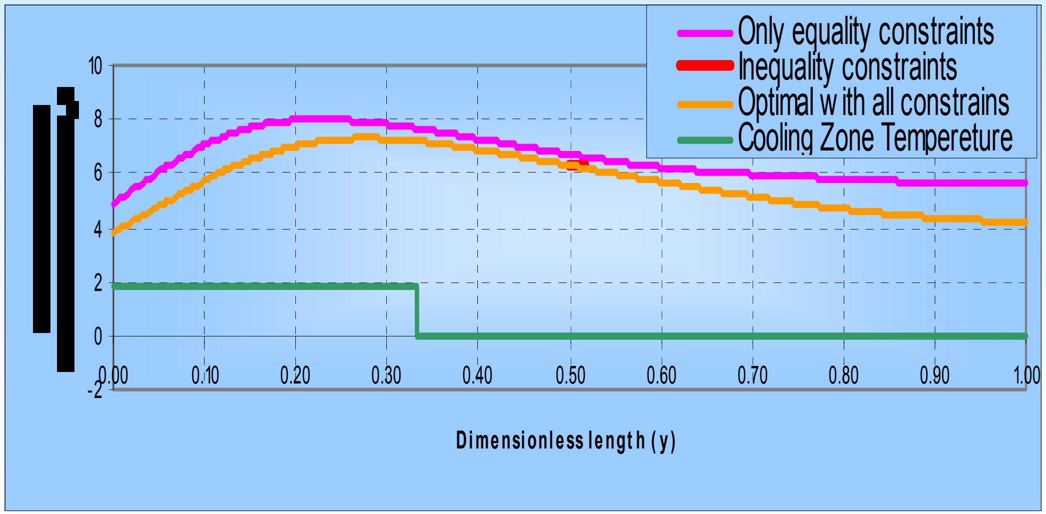
- 12 iterations for convergence
  - 10 iterations for the equality constraints case
- The constraints are active and met
- Optimal values found:
  - $x_{2w,1} = 1.7915$, $x_{2w,2} = 0$, $x_{2w,3} = 0$.
  - Optimal $x_1|_{exit} = 0.9932$



Convergence curve

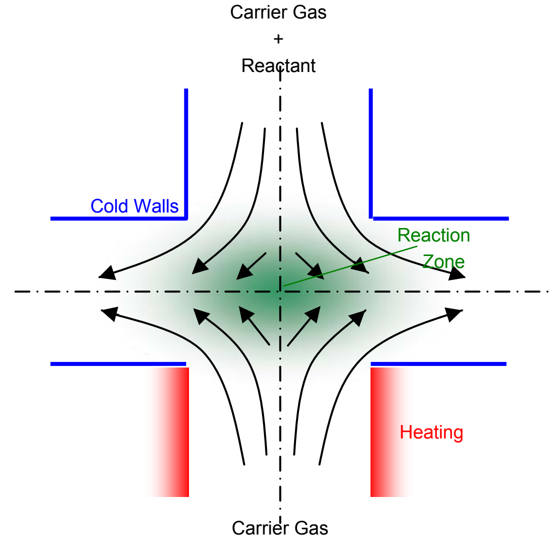


Dimensionless concentration profile for the optimum x_{2w}

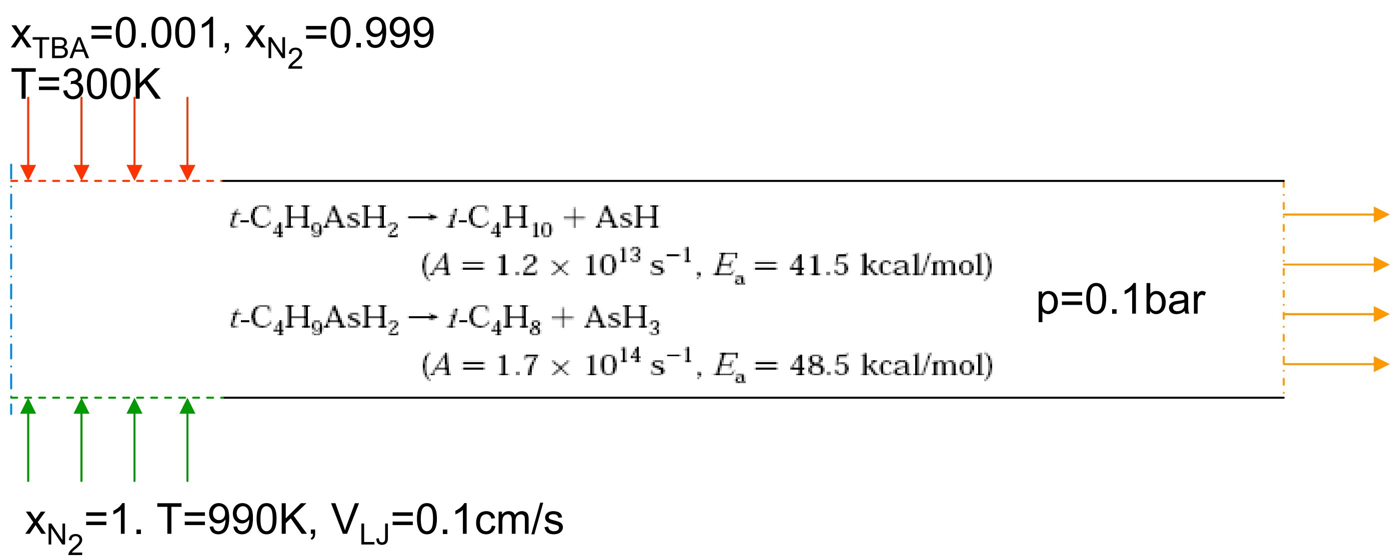


Dimensionless temperature profile for the optimum x_{2w}

Case study II: The counterflow jet reactor



Schematic of the conceptual reactor



Formulation of the model of the counterflow jet reactor

Problem statement:

- maximize the yield of AsH w.r.t. the velocity of the upper stream
  - s.t. the momentum and energy balances are satisfied
- This implies:
  - maximal decomposition of the *tert*-butylarsine (TBA)
  - minimal production of the toxic by-product arsine (AsH_3)

*Safvi, S.A. and T.J. Mountziaris, AIChE Journal, 1994. **40**(9): p. 1535-1548.

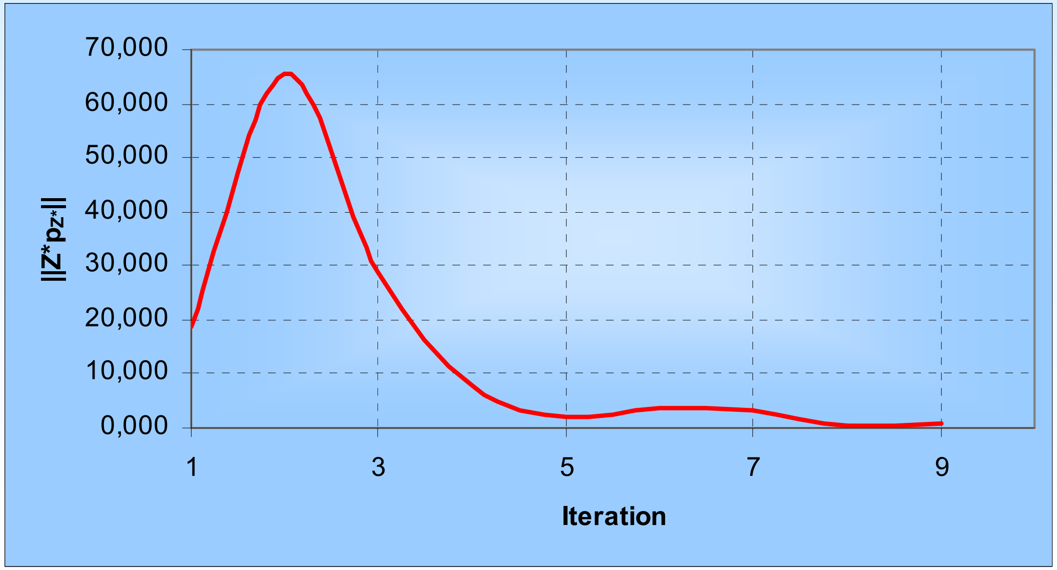
The black-box code

- The model for the reactor was set up using MPSalsa*
- State-of-the-art massively parallel CFD code
  - developed at SANDIA National Laboratories
- Implements the Finite Element Method
  - Unstructured meshes
  - Inexact Newton with iterative linear solvers (GMRES, CG, etc.)
- MPSalsa was used by our optimisation scheme as black-box
- The model of the counter flow jet reactor
  - consists of 19040 dependent variables:
    - temperatures,
    - concentrations,
    - pressures and
    - velocities
  - 1 degree of freedom (the velocity of the upper stream)

* Shadid J, Hutchinson S, Hennigan G, Moffat H, Devine K, Salinger AG, Parallel Computing 1997. 23: 1307-1325

Results

- m=12
- The proposed algorithm converged in 9 iterations
- The optimal inlet velocity found was -0.8193cm/s
- Optimal yield of AsH: 80.34%
- Convergence behaviour:
  - could possibly be enhanced by implementing line searches



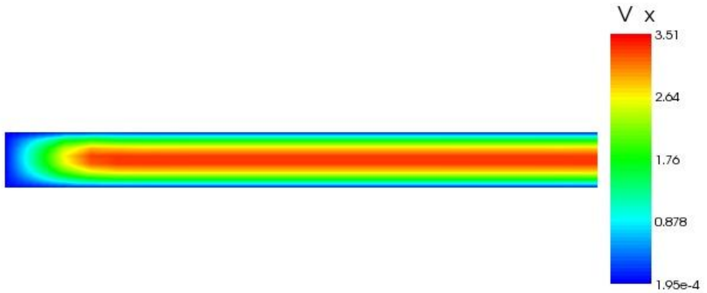
Variable profiles at the optimum

x_{TBA} profile at the optimum V_{US}

x_{AsH} profile at the optimum V_{US}

Temperature at the optimum V_{US}

x_{AsH_3} profile at the optimum V_{US}



x-velocity profile at the optimum V_{US}

y-velocity profile at the optimum V_{US}

Conclusions

- Optimisation framework for large scale steady-state problems
  - Including both equality and inequality constraints
  - With few degrees of freedom
  - Using input/output iterative steady state solvers
- It employs a 2-step projection scheme:
  - Firstly onto the low-dimensional dominant subspace of the system
  - Secondly onto the subspace of the few degrees of freedom
- Only low-order Jacobians and Hessians need to be computed
  - Calculated through few directional numerical perturbations,
  - Good scaling-up with problem size
  - Significant speedup and lower memory requirements
    - in comparison to methods that utilize full Jacobians
- An improved, less expensive version, has also been developed
- This algorithm has been applied for the optimisation of:
  - a tubular reactor where an exothermic reaction A $\rightarrow$ B takes place
  - a counter flow jet reactor for the decomposition of TBA
    - Using a state-of-the art FEM code based on iterative linear algebra solvers

Acknowledgements

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- The financial contribution of the EU Progamme ***CAFE*** [KBBE-212754]

Thank you for your attention!