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Presentation LPT–pre–2001–15

# Dynamic Optimization Using an Adaptive Control Vector Parameterization Strategy

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A. Cruse, W. Marquardt

July 2001

Presented at:
20th IFIP TC7 Conference on System Modelling and Optimization, Trier, 23–27.7.2001.

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# Dynamic optimization using an adaptive control vector parameterization strategy

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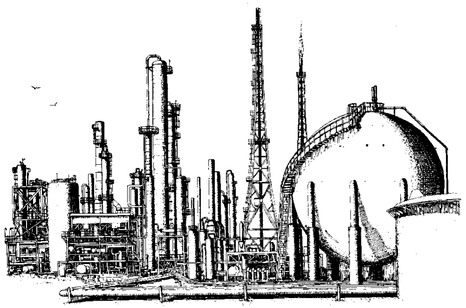
**IFIP 2001, July 27, Trier**

# Motivation

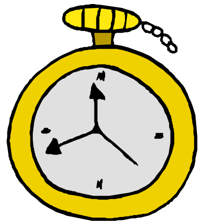
**Dynamic optimization problems** arise in many applications in

- **economics** and
- **almost all engineering disciplines.**

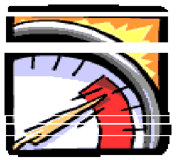
Problems in **chemical engineering** are characterized by:



Highly nonlinear, large-scale
dynamic process models and …



Limited computing time
in real-time applications.



… many path and end point
constraints.

Robust and efficient solution
methods are required.

Generic **dynamic optimization problem** with constraints:

$$\min_{x,u,p} \Phi(x(t_f))$$

$$\begin{aligned} \textit{subject to:} \quad & \dot{x}(t) = f(x(t),u(t),p), \quad t \in [t_0,t_f] \\ & 0 = x(t_0) - x_0, \\ & 0 \le h(x(t),u(t),p), \quad t \in [t_0,t_f] \\ & 0 \le g(x(t_f)). \end{aligned}$$

Necessary optimality conditions lead to multipoint BVPs:

- Highly accurate solutions with shooting techniques.
- Solution requires detailed a-priori knowledge of the optimal solution structure and appropriate estimates for adjoint variables.

Conversion of dynamic optimization problem into NLP by discretization …

… of state and control variables.
(Simultaneous methods,
i.e. Collocation, Multiple shooting)

… of control variables only.
(Sequential method,
i.e. Single shooting)

# Discretization of the time-continuous problem

…too coarse

- Low computational cost
- Low accuracy

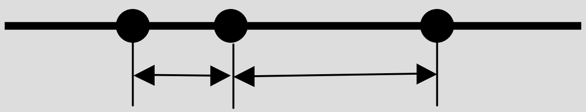
…appropriate

Resolve problem in specified accuracy with minimal degrees of freedom

…too fine

- High computational cost
- Over-parameterization / robustness?

Grid point movement



***Element length as degree of freedom***
(e.g. Biegler *et al*., ‘87, v. Stryk ‘95)

- Introduces nonlinearity and nonconvexity
- Fixed number of grid points

Grid point insertion

***Repetitive insertion of new grid points***

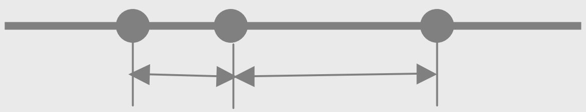
- Grid point doubling (Luus et al., ‘92)
  - No a-posteriori analysis
- Local curvature (Waldraff et al., ‘97)
  - Insertion and deletion
- Error residuals (Betts & Huffman, ‘98)
  - One mesh for controls and states

# Adaptive Discretization

…appropriate

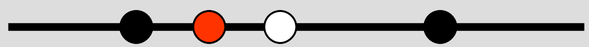
Resolve problem in specified accuracy with minimal degrees of freedom

## Grid point movement



***Element length as degree of freedom***

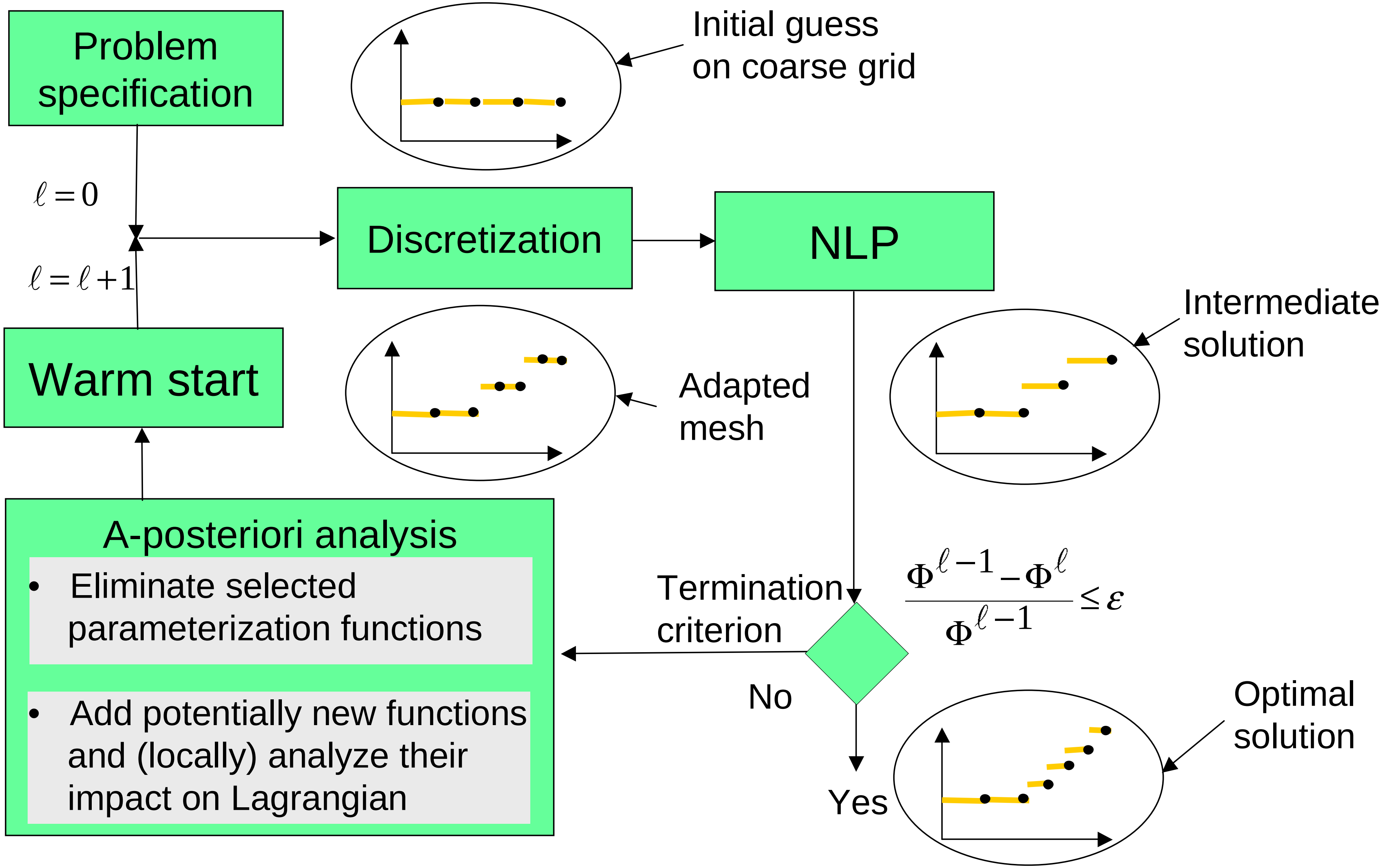
## Grid point insertion and deletion



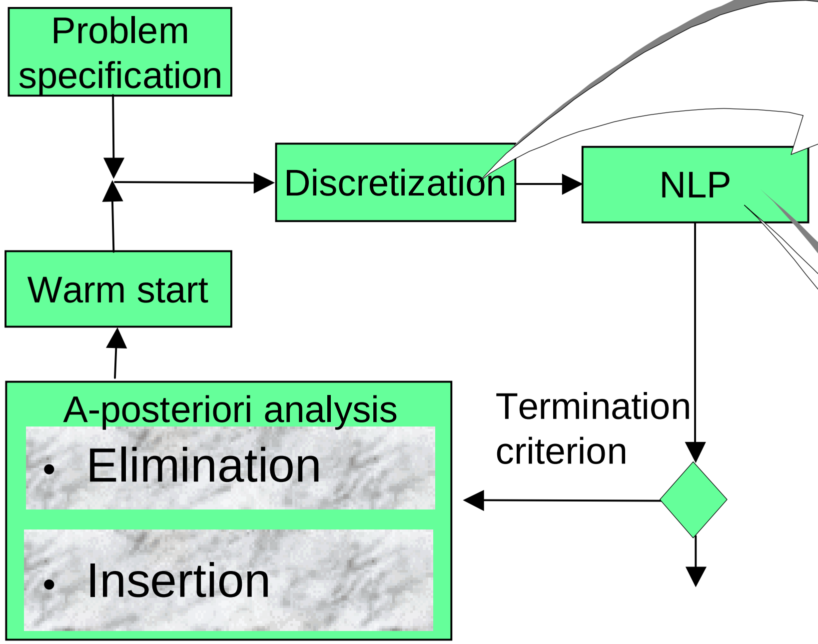
***Repetitive adaptation of grid points based on a-posteriori wavelet analysis***

- Multiple control variables
- Adapted mesh for each control variable
- Lagrangian based refinement

# Framework for adaptation



# Sequential solution approach




Discretization of control variables:

$$u = \sum_{(j,k)\in\Lambda_\varphi} c_{j,k}\varphi_{j,k}(t)$$

Numerical solution of dynamic model as IVP with given initial conditions and controls.

NLP problem formulation:

$$\min_{c_{j,k},p} \Phi(x(c_{j,k},t_f))$$

$$subject\ \ to: \quad 0 \le h(x(c_{j,k}),u(c_{j,k}),p),$$

$$0 \le g(x(c_{j,k},t_f)).$$

Lagrangian: $L = \Phi + \mu_g g + \mu_h h$

**Numerical cost** strongly depends on **discretization** of each control variable.

# Multiscale representation (1)

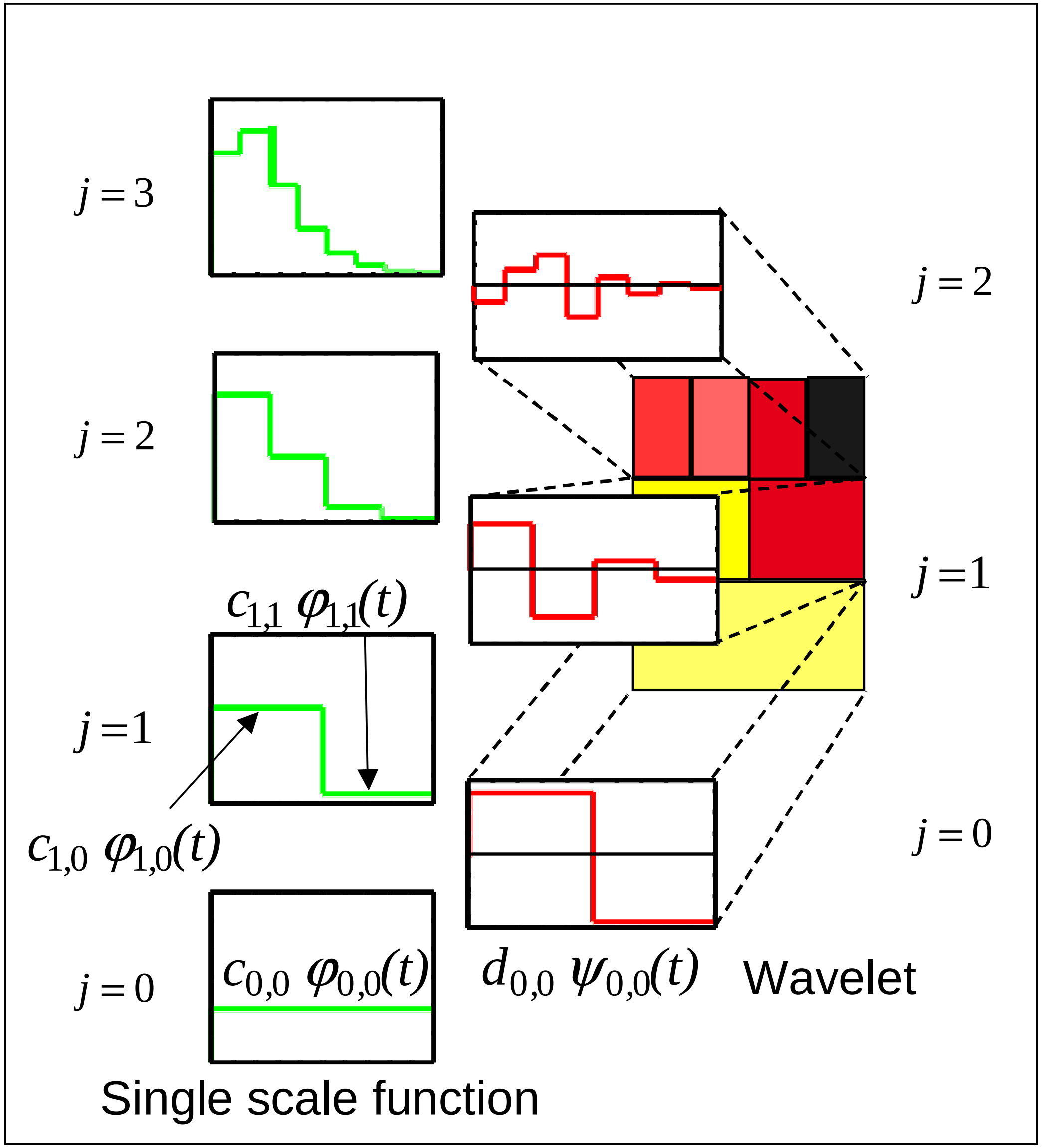
Different **representations** of the **same function …**

… for problem discretization:

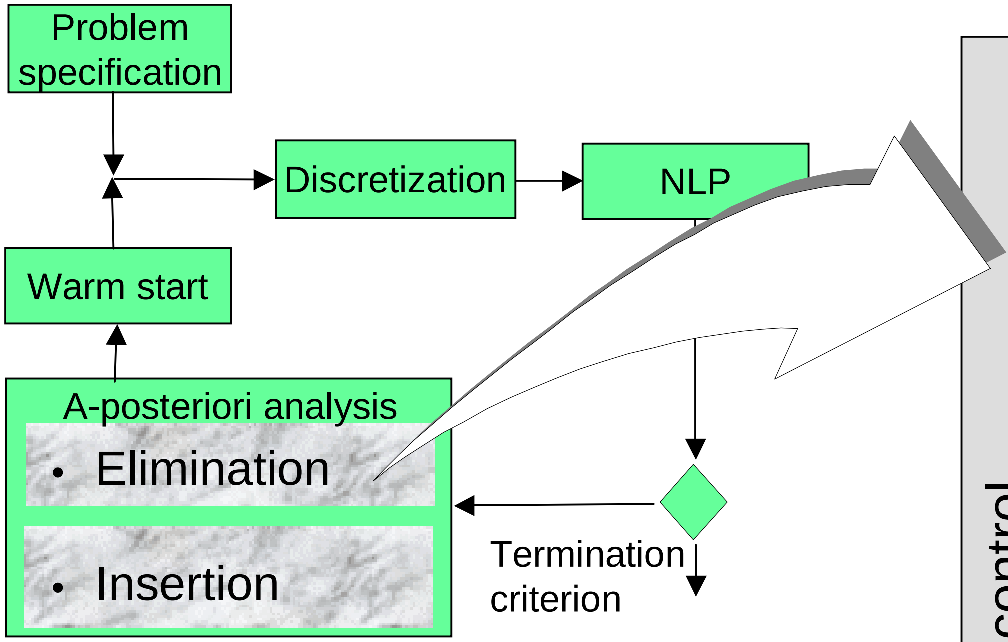
$$u = \sum_{(j,k)\in\Lambda_\varphi} c_{j,k}\varphi_{j,k}(t)$$

… for grid point elimination analysis:

$$u = c_{0,0}\varphi_{0,0}(t) + \sum_{(j,k)\in\Lambda_\psi} d_{j,k}\psi_{j,k}(t)$$



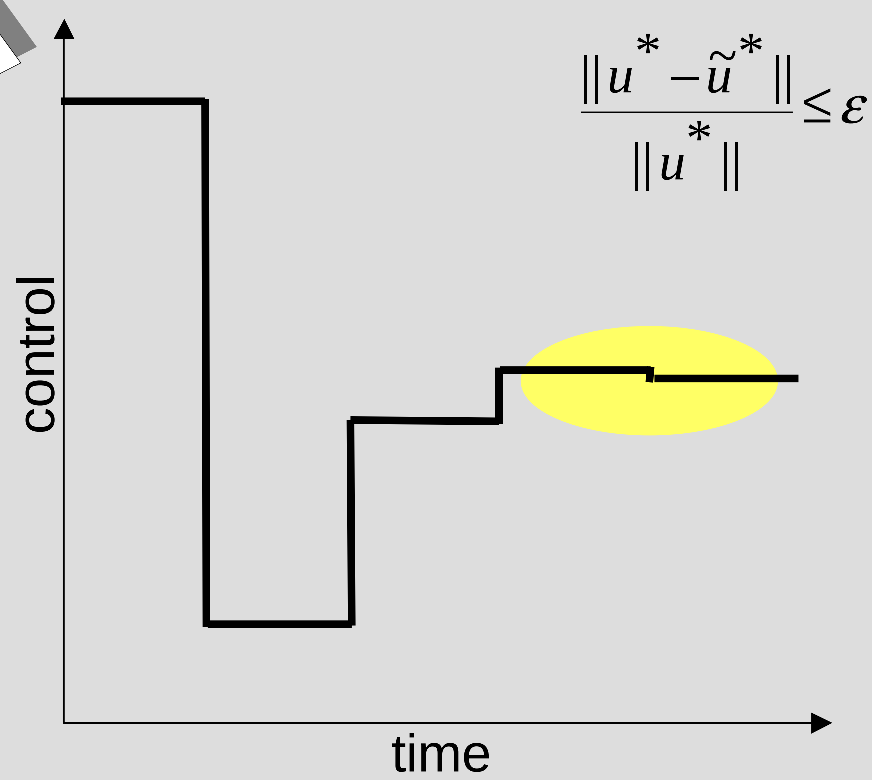
# Elimination of parameterization functions




Analysis of wavelet coefficients of control variables

Minimize number of parameterization functions in $u^*$ such that:

$$\frac{\| u^* - \tilde{u}^* \|}{\| u^* \|} \leq \varepsilon$$




**Approximation:** Norm equivalence $\|u\|_{L_2} \sim \|d\|_{l_2}$ ➡ Discarding small $d_{j,k}$ causes only small changes in approximate representation

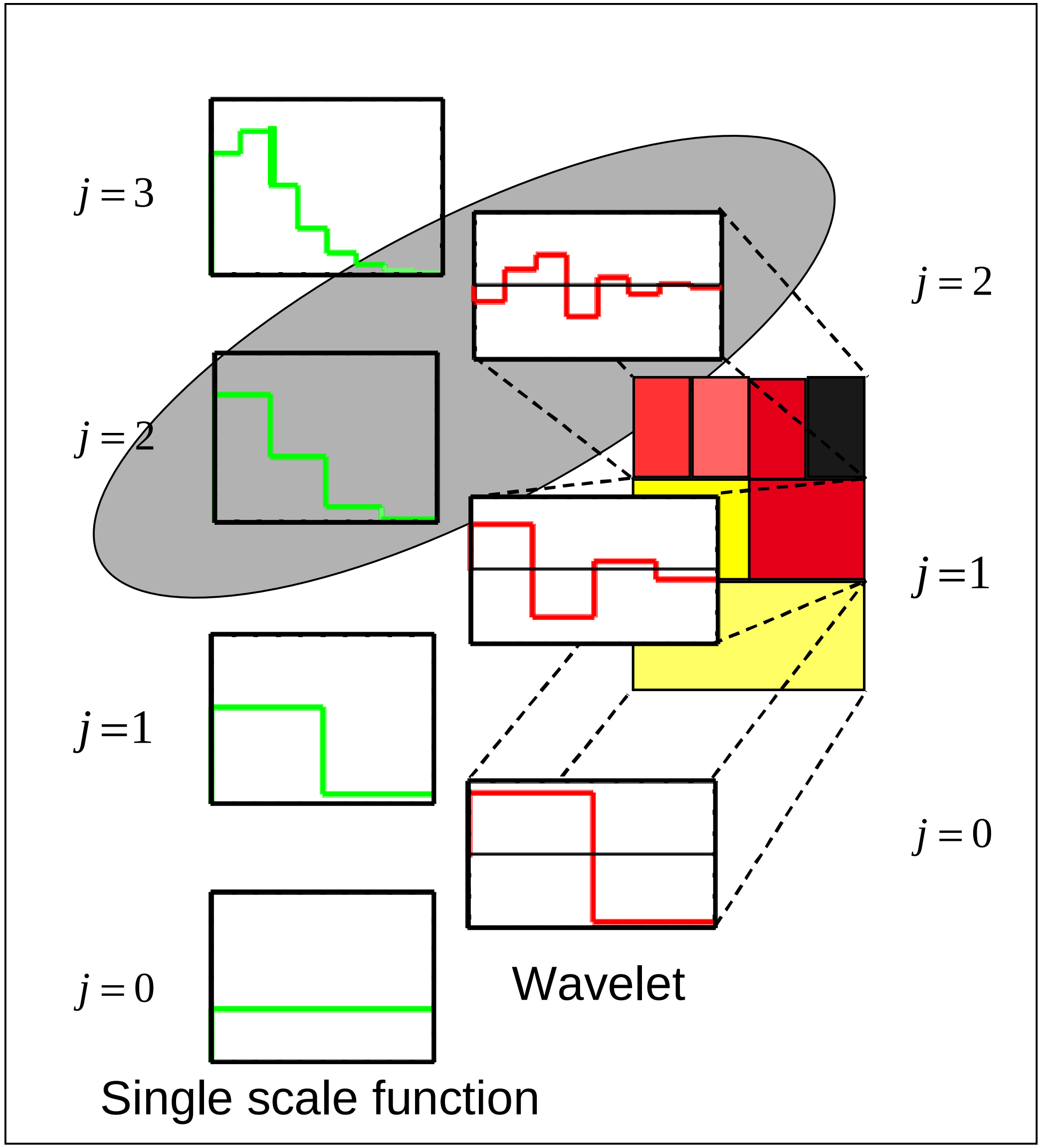
Different **representations** of the **same function …**

… for problem discretization:

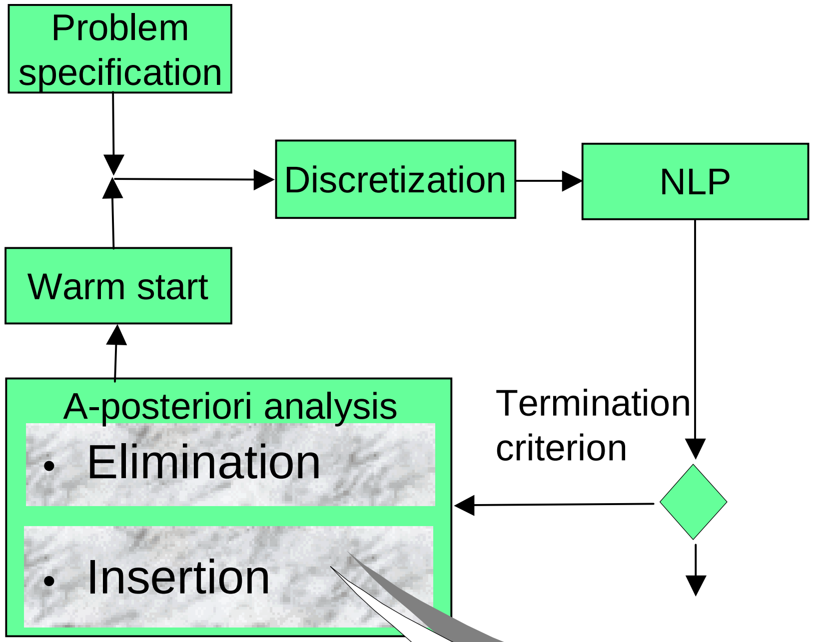
$$u = \sum_{(j,k)\in\Lambda_\varphi} c_{j,k}\varphi_{j,k}(t)$$

… for mesh refinement analysis:

$$u = \sum_{(j,k)\in\Lambda_\varphi} c_{j,k}\varphi_{j,k}(t) + \sum_{(j,k)\in\tilde{\Lambda}_\psi} d_{j,k}\psi_{j,k}(t)$$



# Insertion of new parameterization functions

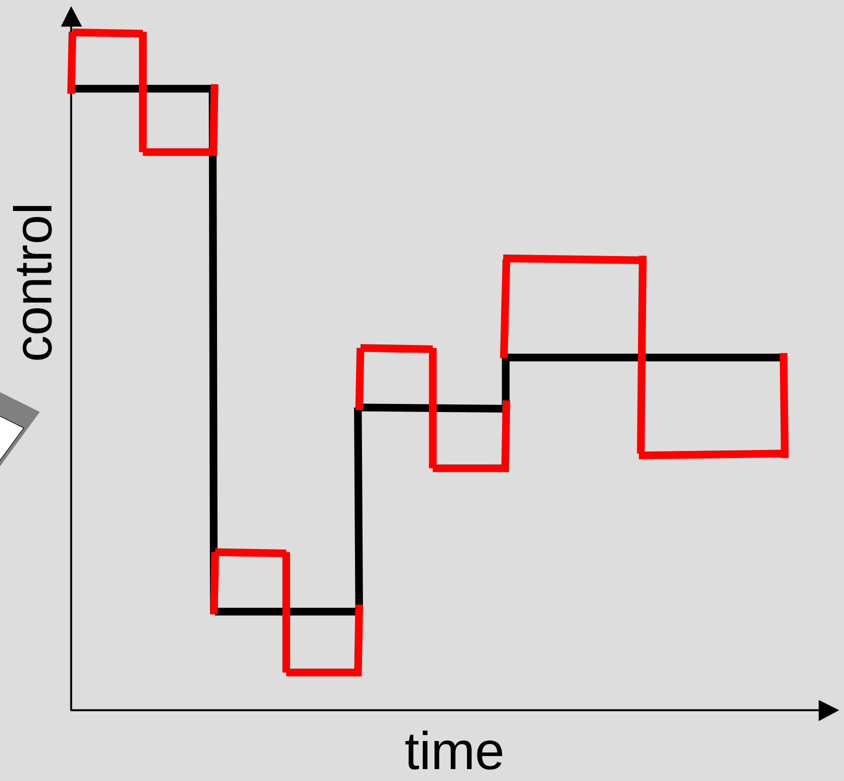



Analysis of a parametric optimization problem in $d_{j,k}$ with $d_{j,k} = 0$.

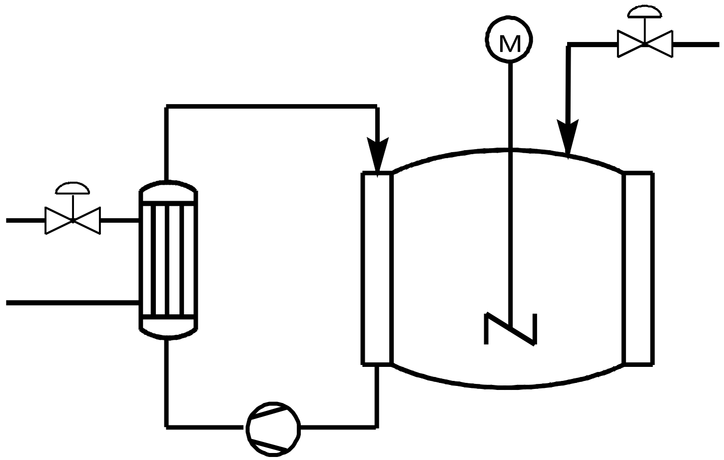
(Büskens, 1998)

Analysis of Lagrangian gradient:

$$\frac{dL}{d\,d_{j,k}} = \frac{d\Phi}{d\,d_{j,k}} + \mu_g^T \frac{dg}{d\,d_{j,k}} + \mu_h^T \frac{dh}{d\,d_{j,k}}$$



# Example: Chylla-Haase benchmark problem




Chylla and Haase, 1993

**Objective:**

- Maintain reactor temperature at $T_r$ (t) = 355 K constant over time

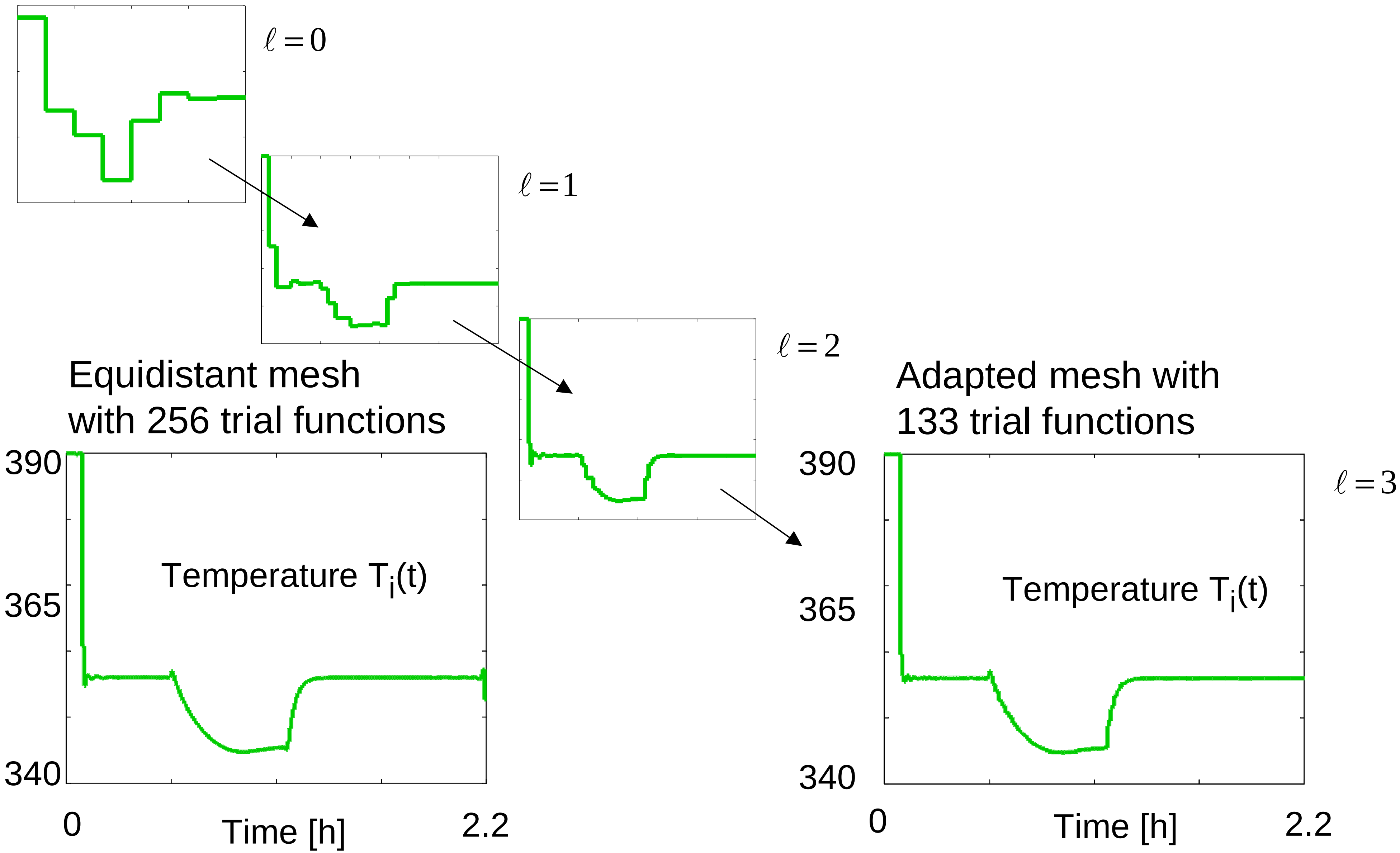
**Control variable:**

- Inlet temperature $T_i(t)$

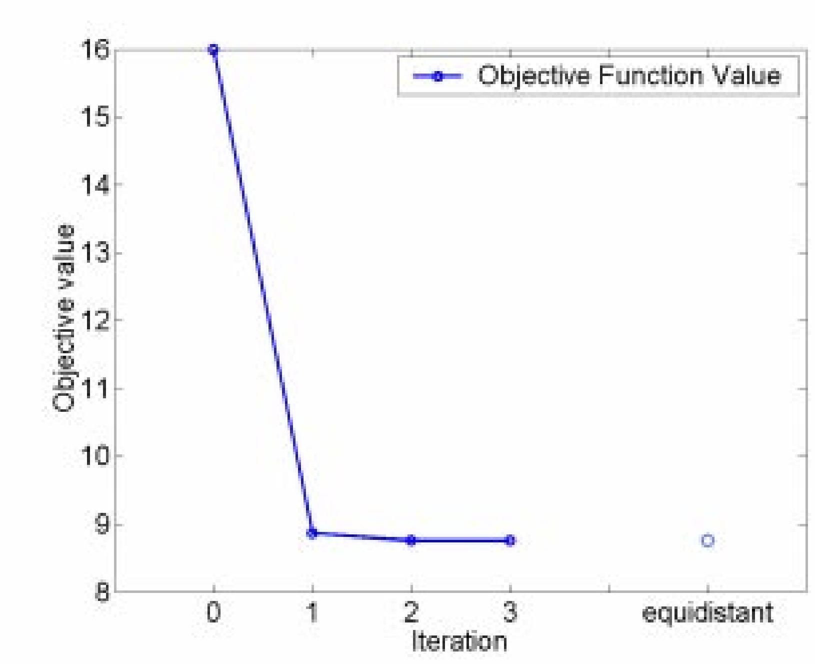
**Dynamic model:**

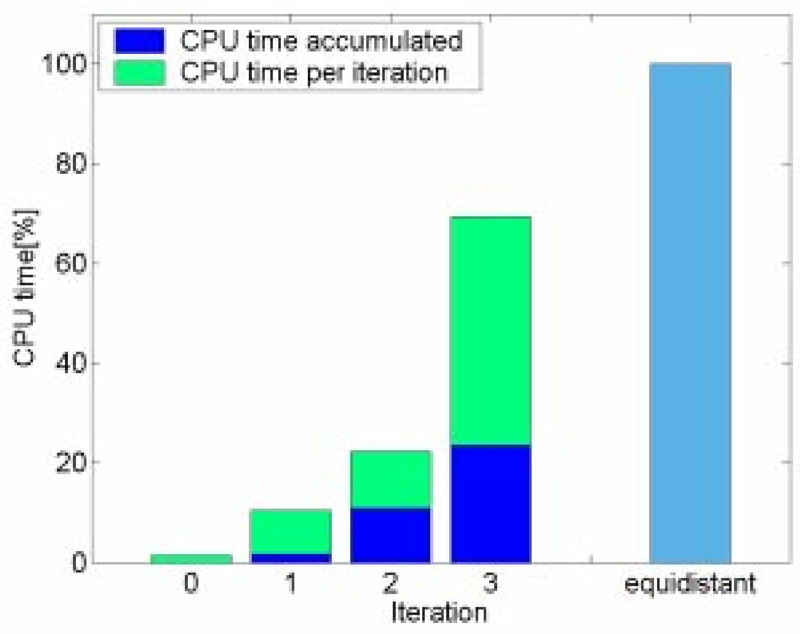
- 31 DAEs (6 differential equations)

# Results: Chylla-Haase reactor

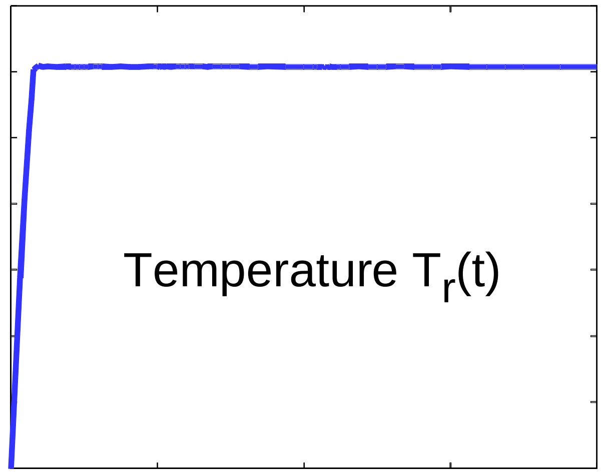


# Results (2): Chylla-Haase reactor

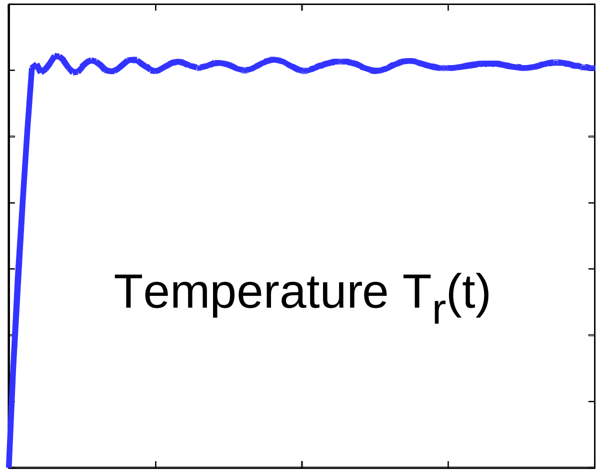


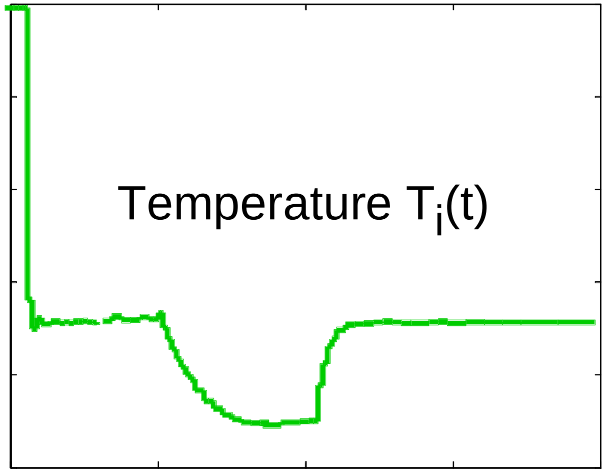



# Effect on robustness?

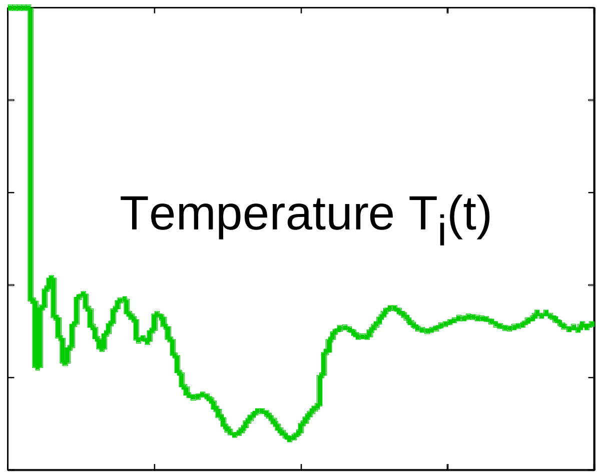



Unscaled model,
low tolerances



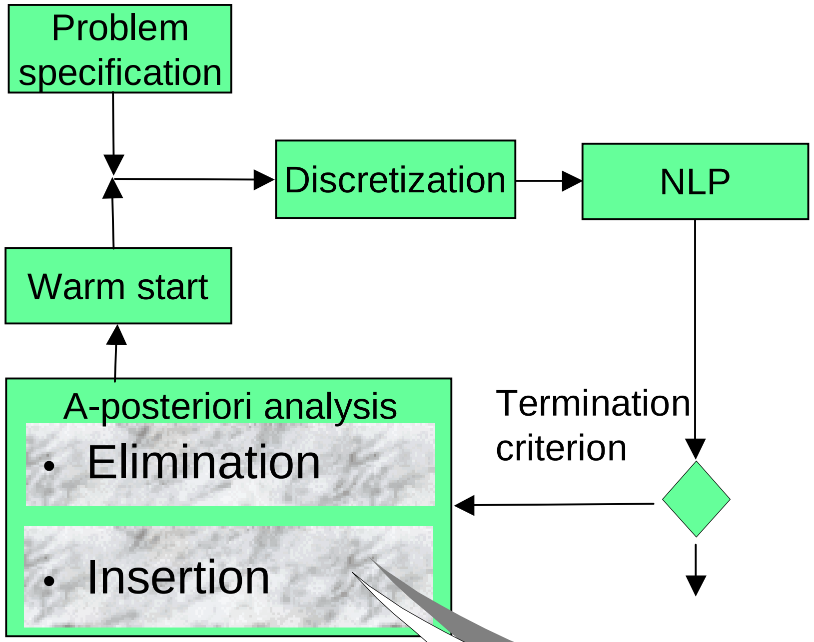

Lagrangian based adaptation leads to **inherent scaling** of the gradients



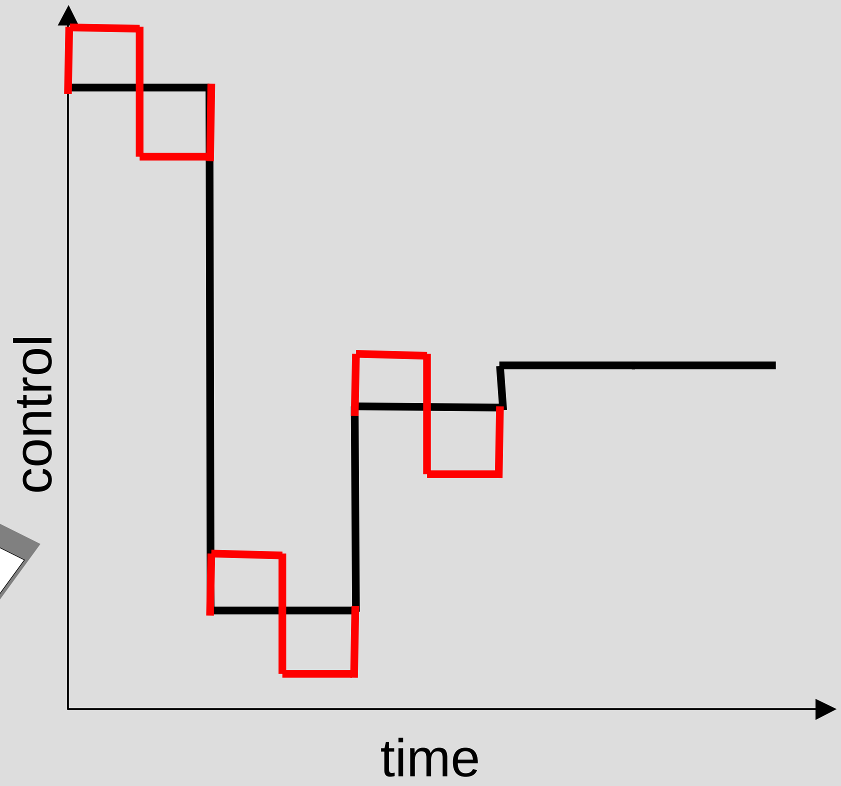

Optimal profiles with repetitive grid adaptation

Optimal profiles with highly resoluted, equidistant mesh

# Insertion: An alternative approach

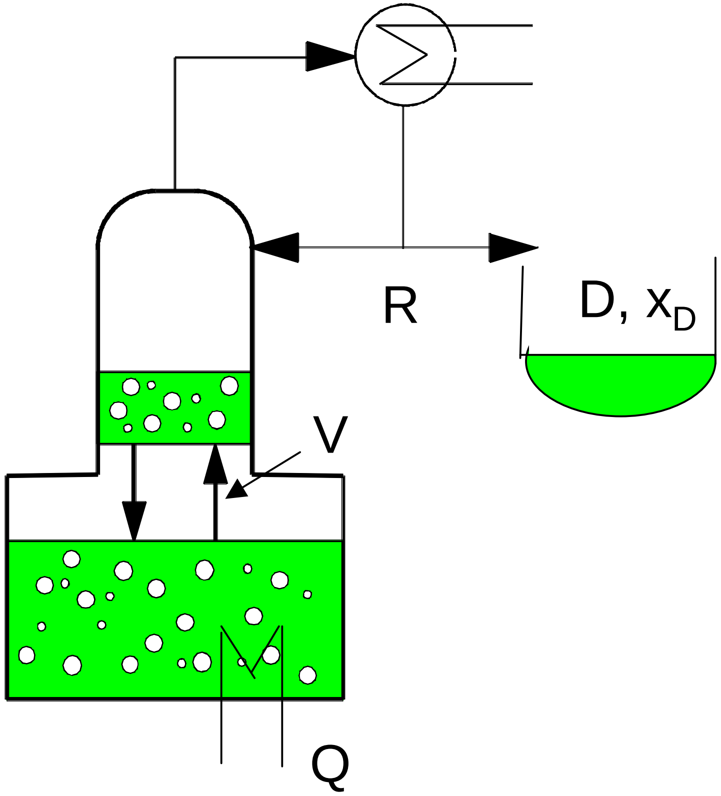



Introduction of new parameterization functions where $\|d_{j,k}\| \geq \eta$




Analysis of wavelet coefficients of control variables

# Example: Batch reactive distillation




**Objective:**

*Minimize energy demand* with given:

- Fixed batch time
- Amount of distillate $D \geq 6.0$ kmol
- Product purity $x_D \geq 0.46$

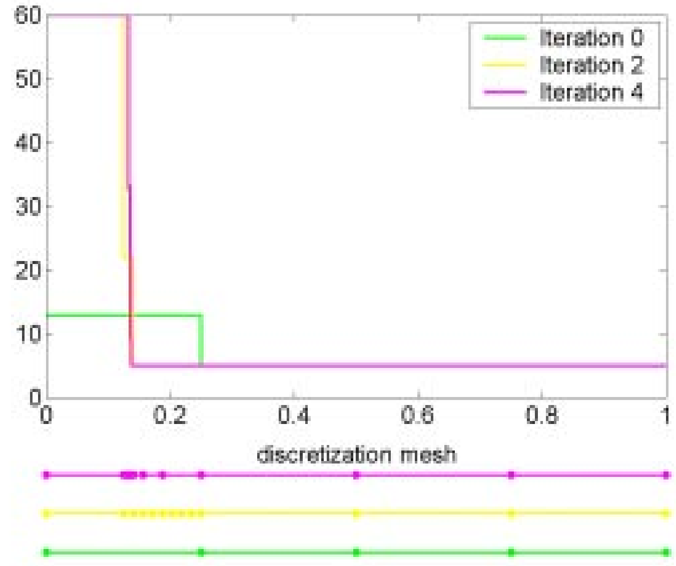
**Controls:**

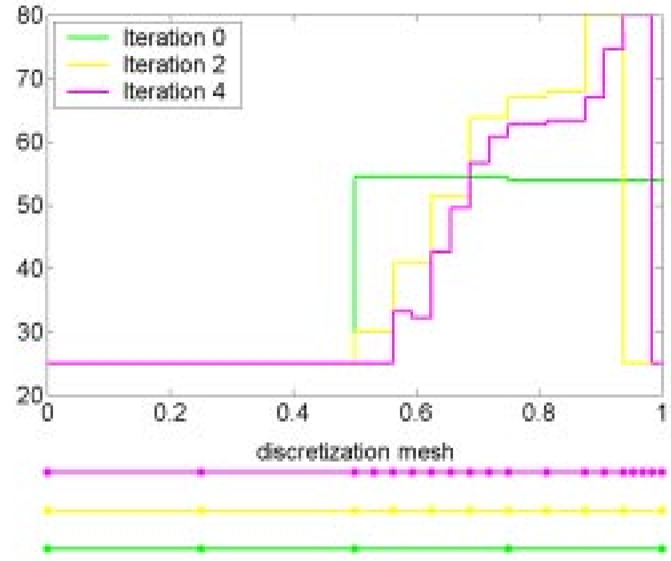
- Reflux ratio R(t)
- Vapor rate V(t)

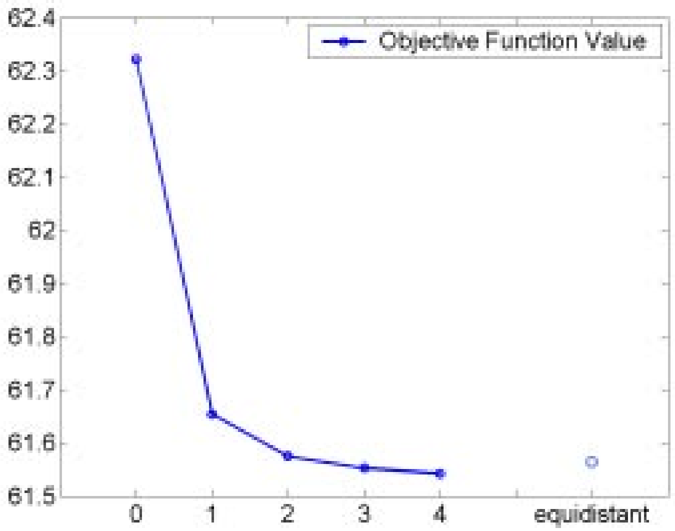
**Dynamic model:**

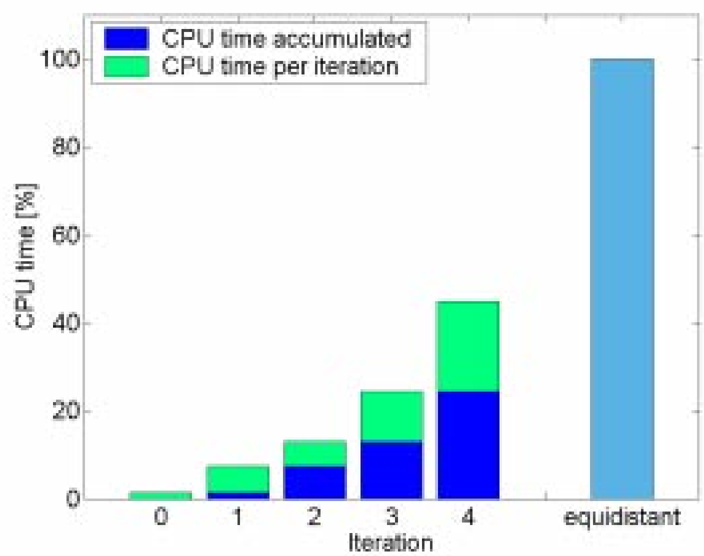
- 10 theoretical trays
- gPROMS model contains 418 DAEs (63 differential equations)

# Results: Batch reactive distillation

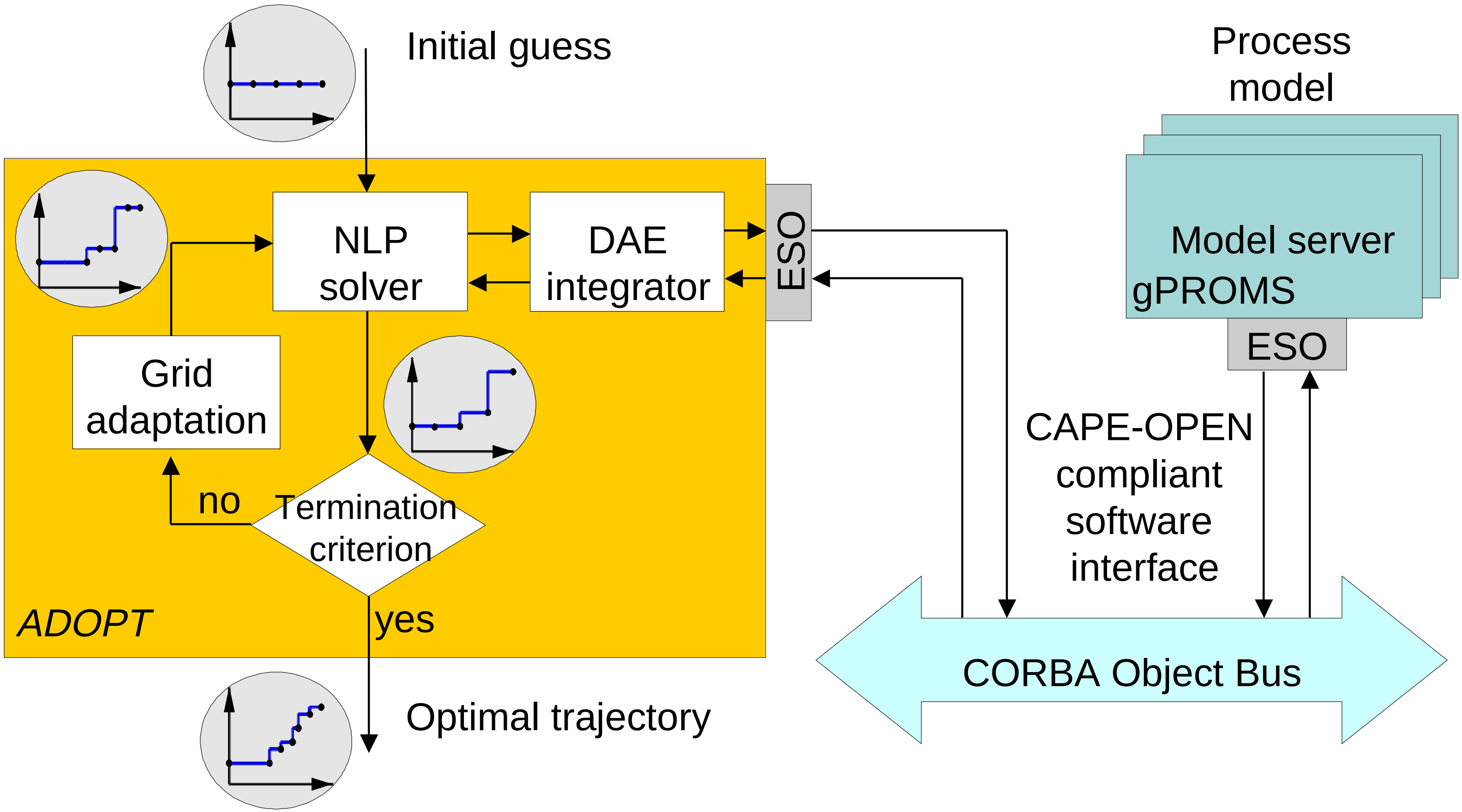


# Software implementation



# Conclusions

**Adaptive discretization strategy** for solving dynamic optimization problems:

- Applicable to **general constrained optimization problems.**
- Reduced overall **numerical cost.**
- Improved **robustness** through gradient *scaling*.
- Intermediate solutions are suboptimal but **feasible.**

**Future work**:

- **Higher order** parameterization functions.
- Improvement of **warm start** functionality.
- Better understanding of refinement strategies / Appropriate threshold tolerances.