Hybrid modelling and model reduction for control & optimisation

based on research done by
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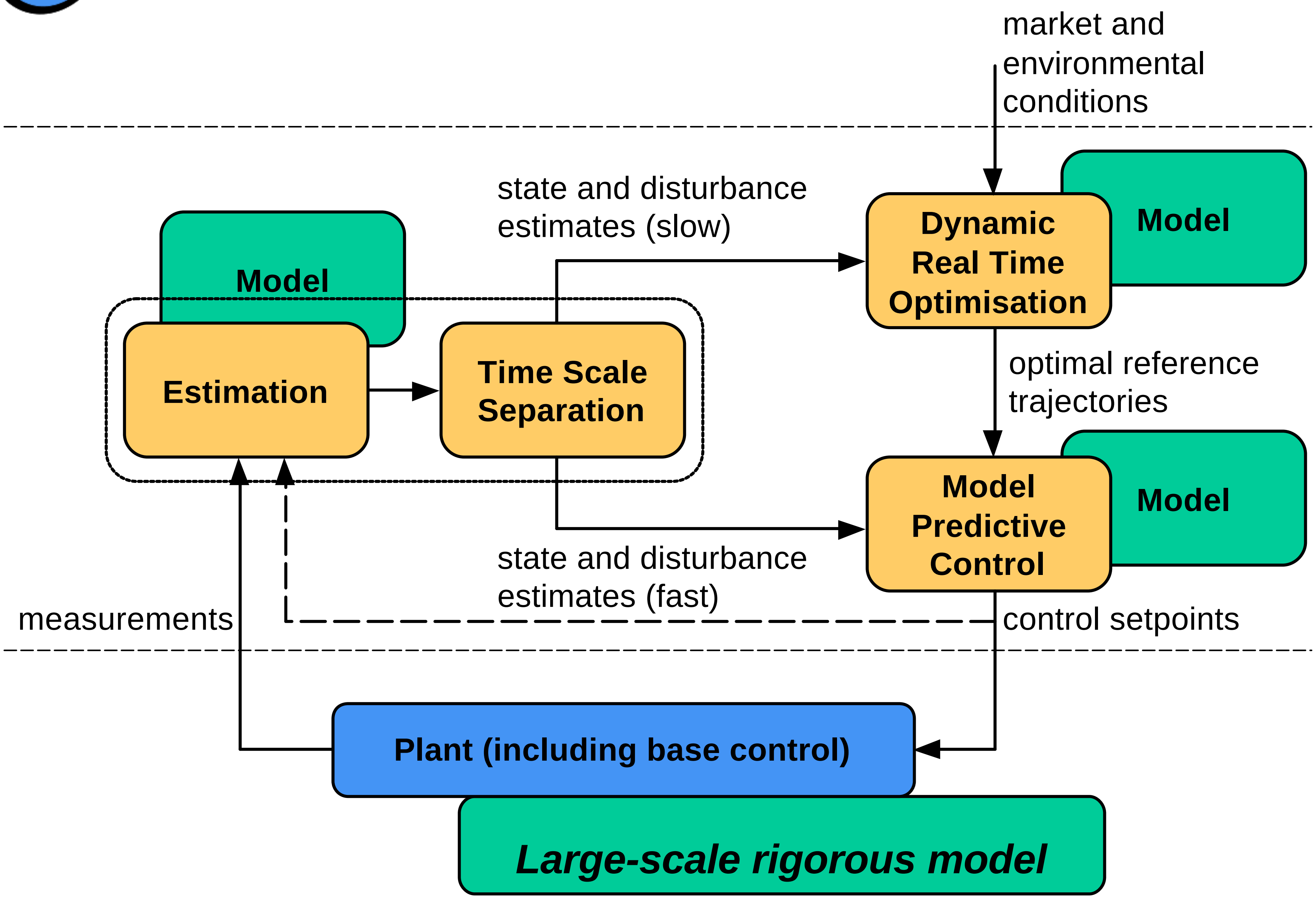
Models for control and optimization



Contents

* Large scale physical modeling
* Hybrid components
* Physical based complexity reduction
* Mathematical complexity reduction
* Application aspects for INCOOP tasks
* Conclusions

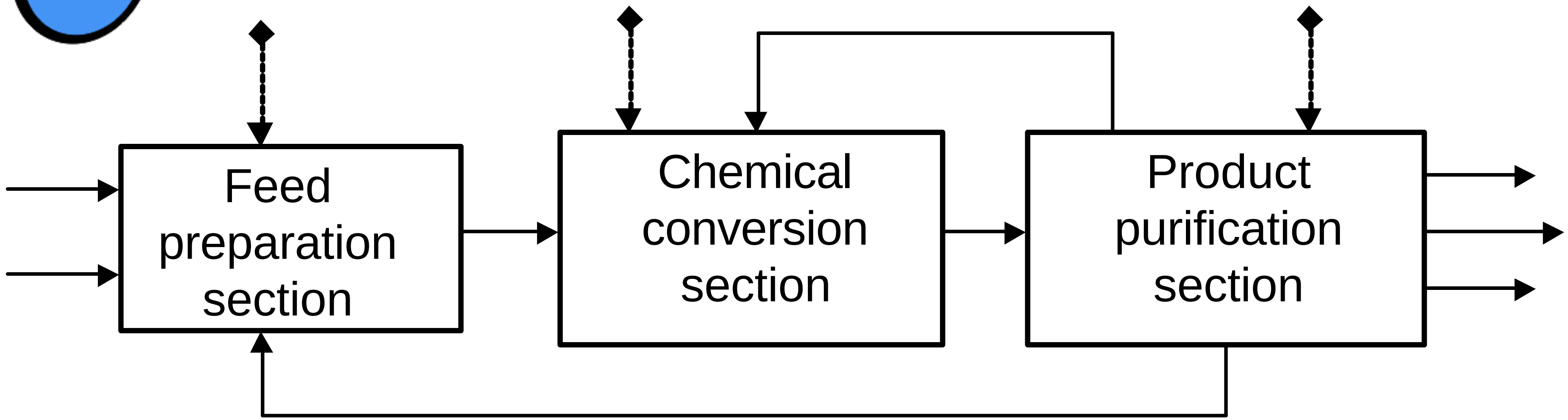
Plant operations modelling:

- *process with sensors and actuators* ☯
- *conventional controllers* ☯
- *external disturbances* ☯
- operating window constraints -
- economical objectives -

Aspects of modelling:

- *technology of modelling* ☯
- mainly generic aspects ☯
- specific aspects: see Bayer and Shell applications
- work processes underexposed

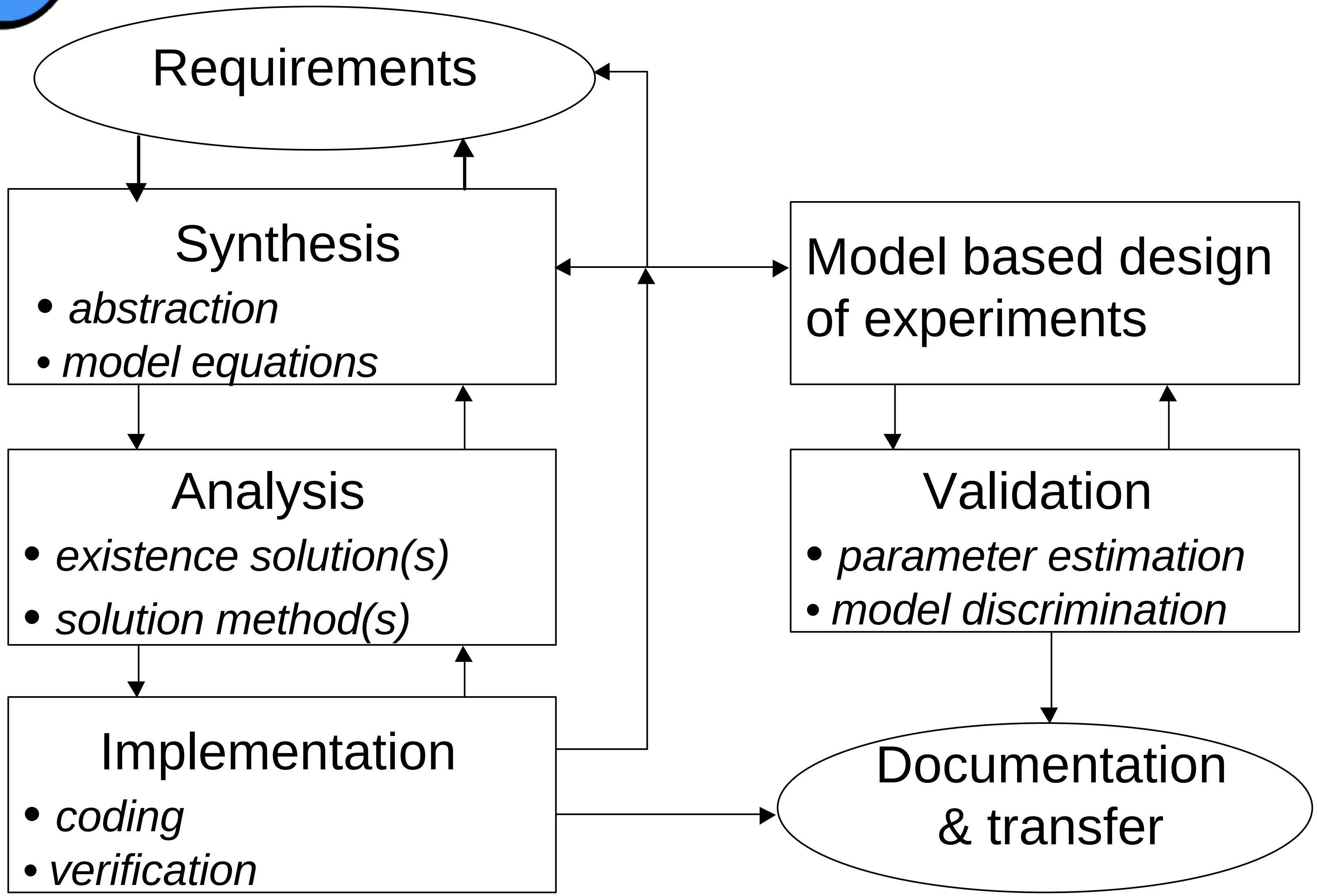
LSM: plant features



- multiple modes of production + switching
- disturbances
- multiple units / section & many compartments / unit
- recycling & heat integration
- non-linear behaviour (units + plant wide integration)
- very wide range of relevant time scales (μs - days)
- several thermodynamic phases with many species

=> Large scale dynamic process models (10^3 - 10^5 DAE's)

LSM: Systematic model development



LSM: functional requirements

Aim: accurate representation of physical behaviour:

- *relevant time scales* => how small ?
- *feasible operational window:*
  - * *physical ranges of inputs, states, outputs*
- *for realistic disturbance scenarios*

Trade-off's:

- *complexity vs costs of development & validation*
- *complexity vs maintenance (costs)*
- *in closed loop: complexity vs accuracy*

Abstraction:

from reality to a modelling space with bounds:

- objects: *contents and walls of equipment, streams, sensors, controllers, actuators, ..*
- spatial resolution: *mixed compartments, distributed in n-D.*
- time resolution: *continuous, discrete*
- chemical species: *discrete, continuous*
- thermodynamic phases: $V, L_1, L_2, S_1, S_2, ..$
- chemical reactions: *discrete, continuous;*
- states of particles: *size, stress, charge, ..*
- …..

Key issue: how to find relevant level of detail

LSM: Structure of unit models

Ψ

$\mu_k^{(\alpha)} = \mu_k^{(\beta)}$

$$\partial\,(m.a)/\,\partial\, t \quad = \sum_n F^{(n)}\,.a^{(n)} + \Psi_{(dif.)}(a) + R(a)$$

F

Model equations:

- conservation / change: *truly first principles*
- thermodynamic states: a=a(P,T,c)
- transfer rate: $\Psi = \Psi\,(\nabla P,\ \nabla T,\ \nabla c)$, $F=F(\nabla P)$
- source/sink rates R=R(P,T,c)
- phase equilibria $m_k^{(a)} = m_k^{(b)}$, $T^{(a)} = T^{(b)}$

LSM: Physical properties & thermo

Equations for:

- thermodynamic variables per species and per phase:

  density, specific heat, entropy, enthalpy, free enthalpy

- transport coefficients:

  viscosity, heat diffusion, species diffusion, surface tension

- Needed information:

  variables: $P_k(p_k^{(0)},P,T;par_k)=0$ and $p^{(\alpha)}=P^{(\alpha)}(P,T,x,p^{(0)})$

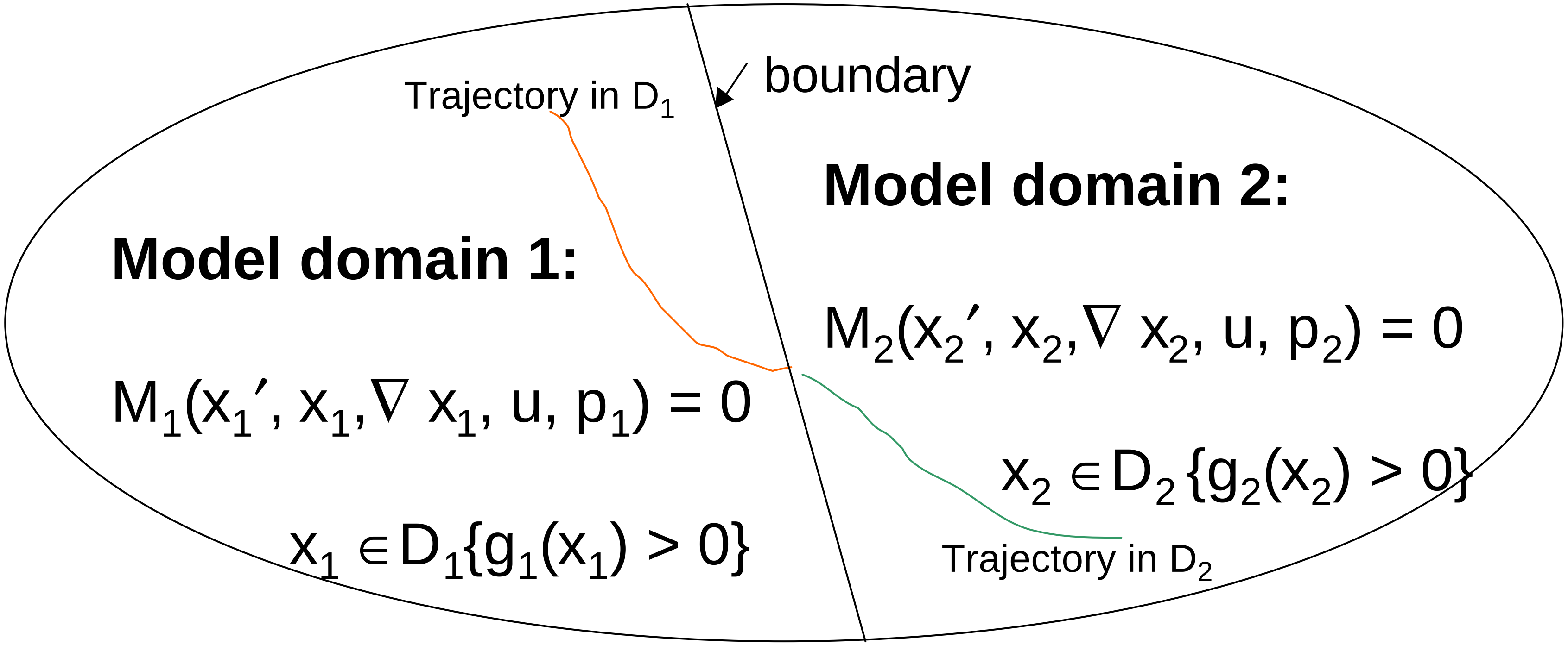
  gradients: $\partial p / \partial q = \partial P(P,T,x) / \partial q$ with $q=\{P, T, x\}$

- Issues:

  models in “closed” software box

  computational speed & accuracy of solution ?

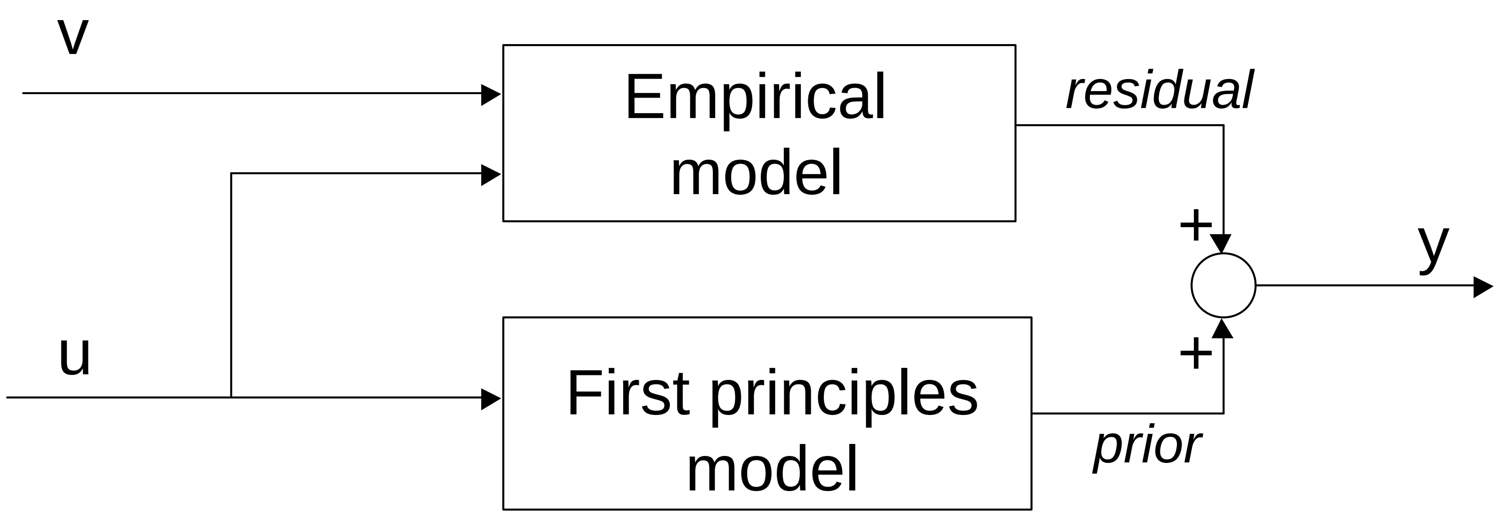
LSM: Transitions between models



Transition:	*e.g. phase split*	
State event:	$g_1(x_1) = 0$	if approaching from D_1
	$g_2(x_2) = 0$	if approaching from D_2
Continuity:	$T(x_1, \nabla x_1, x_2, \nabla x_2,) = 0$	

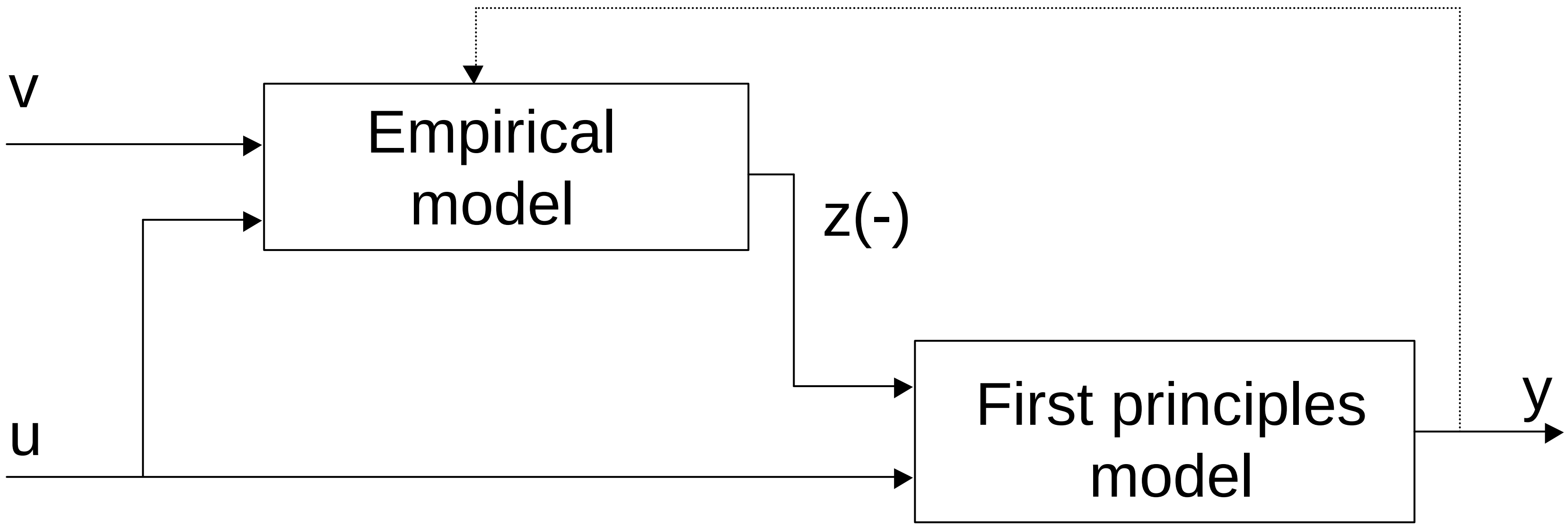
Hybrid models comprise first principles as well as empirical components to deal with uncertainty or complexity.

Parallel structure: ad-hoc model error compensation



LSM: Sequential hybrid model

Sequential structure: physically motivated extension



Empirical modelling:

- static (non-linear) regression model; e.g. ANN, $z = z(\pi, v, u, y)$
- dynamic trend model: $z(t) = z(\pi, v, u, y)$ with $\pi' = 0$; update of π

LSM: Hybrid, empirical components

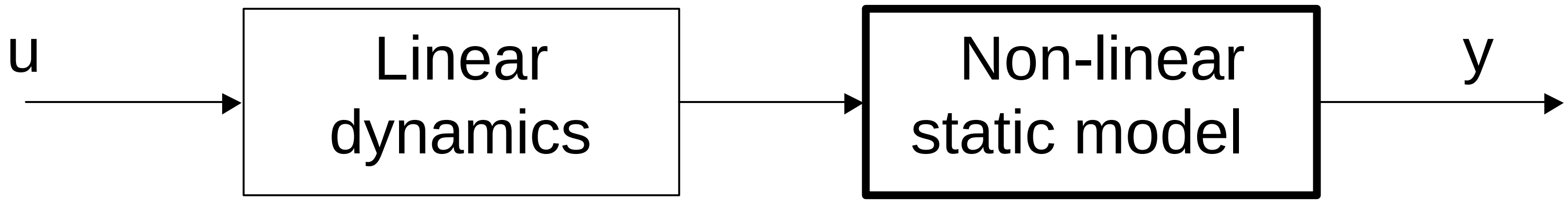
Requirements to empirical components in combination with physical modelling:

- continuous and differentiable (bounded) in all variables
- comply with correct physical asymptotic behaviour:
  - $\partial x / \partial t$, $\nabla x \geq 0$ for $x \downarrow 0$ when $x \geq 0$; e.g. **not** $dc / dt = k.c^{-a}$ (a>0);
  - no fluxes remain when forces vanish; equilibrium conditions
- no introduction of spurious roots
  - e.g. rate = $k_1.c /(1+k_2.c + k_3.c^2)$
  - second order term in denominator may enhance fitting accuracy but it creates a maximum in the rate, allowing for multiple solutions.

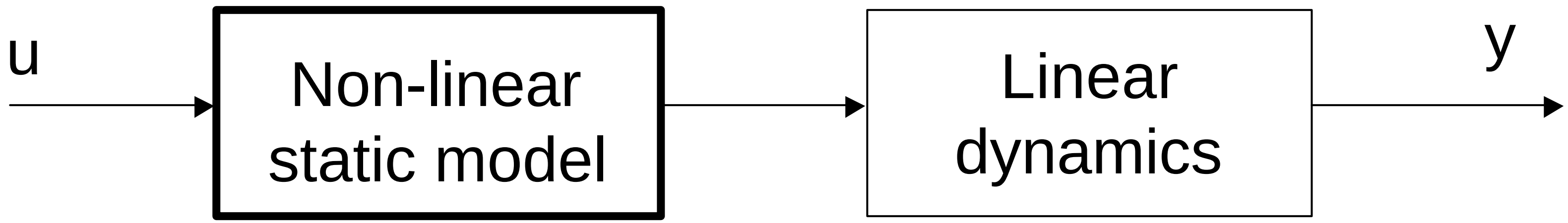
LSM: Wiener / Hammerstein hybrid models

- static fundamental model available (process simulators)
- plant dynamics accessible by plant tests (linear models)

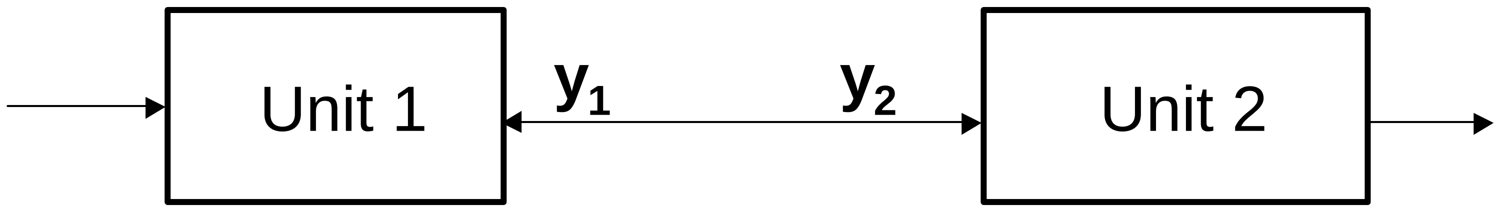
Wiener structure:



Hammerstein structure:



LSM: Linking of unit models



Connectivity conditions: $f \equiv y_1 - y_2 = 0$

Physical consequences of coupling (mass / heat):

- *recycles increase I/O time constants:* $T = \sum_i \tau_i / (1 - \prod_i K_i)$
- *can induce non-linear, positive feedback:*

  => multiple stationary states can occur

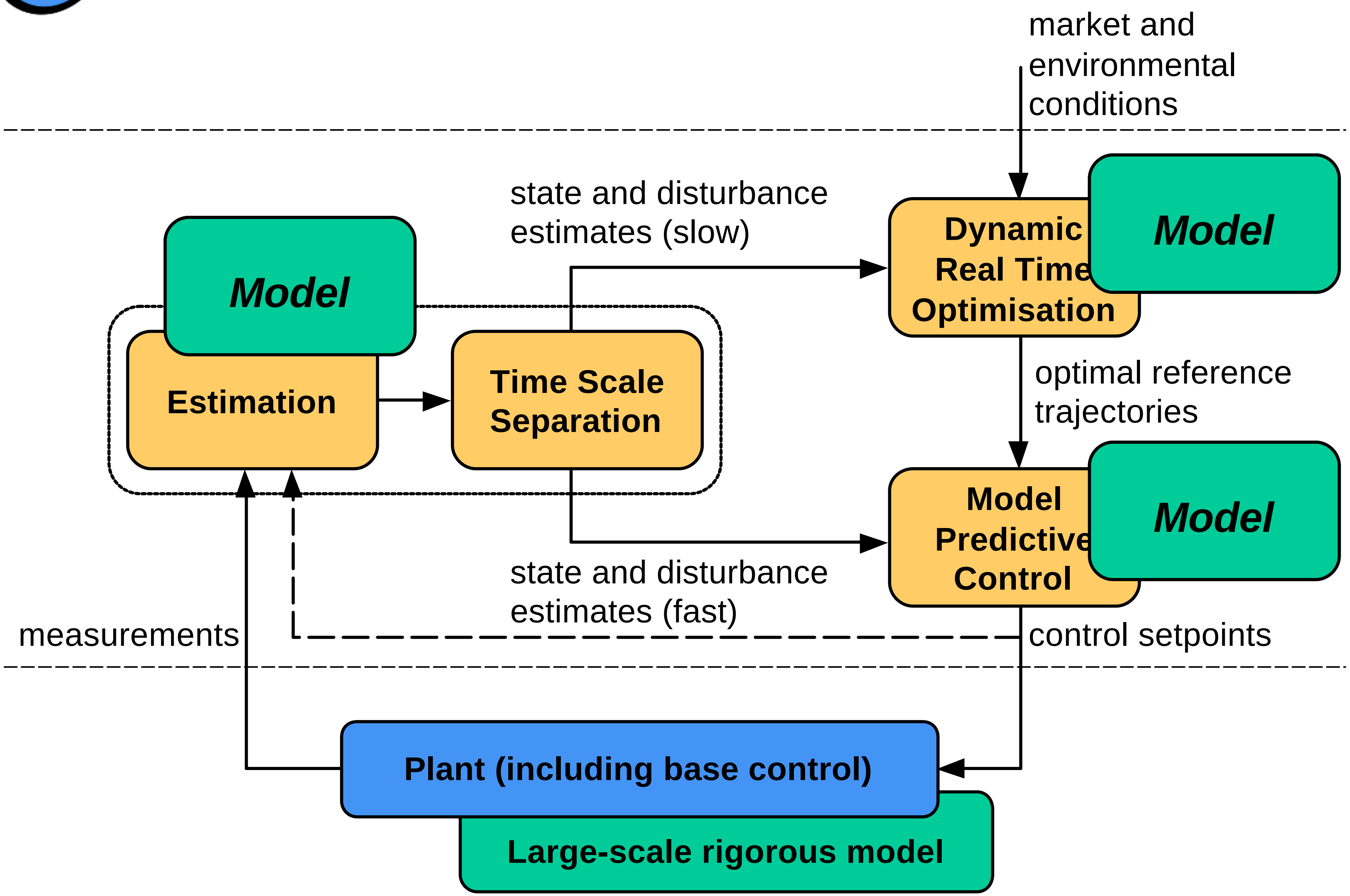
LSM: Wrap - up

- Focus has been on model synthesis
- Structured approach is essential to reduce modelling errors
- Decomposition / aggregation at the finer scales ?
- Model synthesis more an art than a science

- Not covered: many other important aspects
  - *differential index problems*
  - *scaling and initialisations of DAE's*
  - *global sensitivity analysis*
  - *experimental validation aspects*

Large scale plant model will now serve as 'source' model for reduction to models suitable for on-line use in control and optimisations

Models for control and optimization



Options for reduction:

- reduce the modelling space
  - lumping of species, reactions, phases
  - combining compartments, lumping by OCFE
  - …
- simplify equations (structure):
  - by linearisation;
  - (non-linear) approximations of complex expressions; e.g for physical properties and kinetics
- reduce number of equations / order reduction
  - remove trivial linear connectivity equations and variables
  - order reduction

Model simplification: elimination connectivities

Modular modeling (e.g. in gPROMS)

- ⇒ large number of redundant equations of type X = Y (e.g. connection of different trays in distillation column)
- ⇒ increased model size without additional physical information

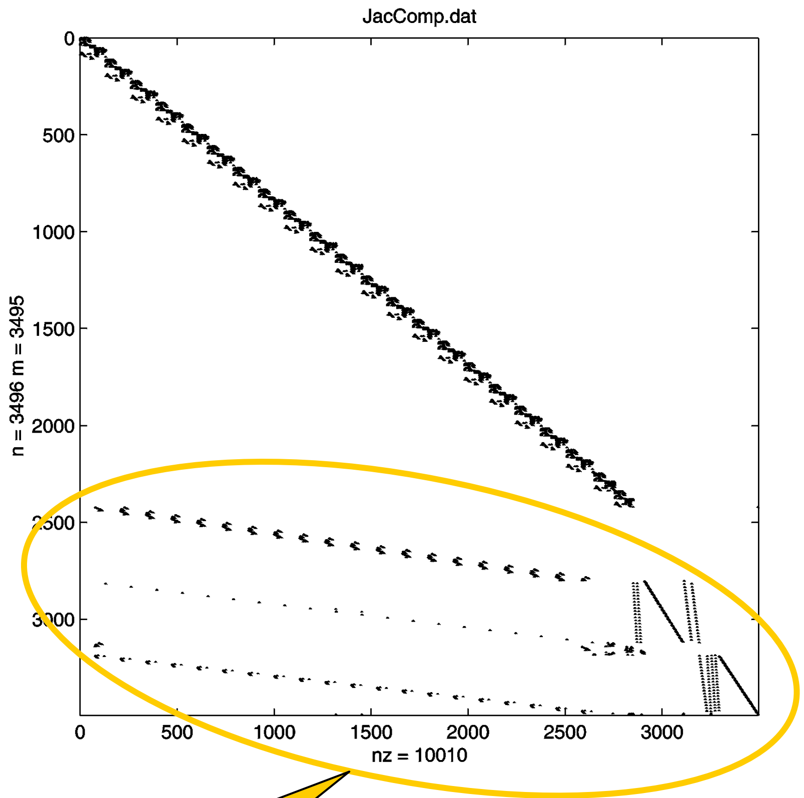
Idea:

- ⇒ Determine redundant equations and variables by automatic analysis of the system‘s incident matrix
- ⇒ Perform automatic mapping of variables in simulation /optimization software

Prototype

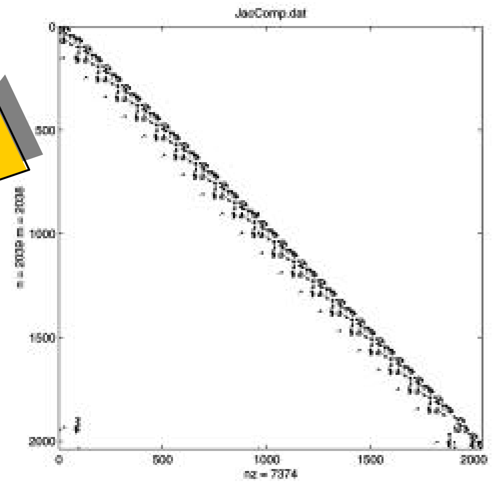
- ⇒ Implemented in sequential approach dynamic optimization software

Application to distillation column I



Redundant equations

Simplification procedure



- Model size reduced from 3496 to 2039
- Computation time in optimization reduced by 53%

Singular perturbation: $\dot{x}_2 = 0$

$$\begin{aligned} \dot{x}_1 &= f_1(x_1, x_2, u) \\ \dot{x}_2 &= f_2(x_1, x_2, u) \end{aligned} \quad \Rightarrow \quad \begin{aligned} \dot{x}_1 &= f_1(x_1, x_2, u) \\ 0 &= f_2(x_1, x_2, u) \end{aligned}$$

Truncation: $x_2 = c$

$$\begin{aligned} \dot{x}_1 &= f_1(x_1, x_2, u) \\ \dot{x}_2 &= f_2(x_1, x_2, u) \end{aligned} \quad \Rightarrow \quad \begin{aligned} \dot{x}_1 &= f_1(x_1, c, u) \\ c &= x_2 \end{aligned}$$

Example of singular perturbation

Batch reactions:

(slow): B + **C** <=> D

(fast): **A** + D <=> B + **E**

Model:

$$c_A' = \qquad\quad - r_2$$
$$c_B' = -r_1 + r_2$$
$$c_C' = -r_1$$
$$c_D' = +r_1 - r_2$$
$$c_E' = \qquad\quad + r_2$$

$$r_1 = k_1(c_B.c_C - c_D / K_1)$$
$$r_2 = k_2(c_A.c_D - c_B.c_E / K_2)$$
$$k_2 = k_1 / e$$

Transform model to separate fast and slow modes

$$\xi_1' = r_1$$

$$\xi_2' = r_2 \quad => e.\,\xi_2' = \underline{r}_2$$

$$c_A = c_A^0 \qquad\quad - \xi_2$$
$$c_B = c_B^0 - \xi_1 + \xi_2$$
$$c_C = c_C^0 - \xi_1$$
$$c_D = c_D^0 + \xi_1 - \xi_2$$
$$c_E = c_E^0 \qquad\quad + \xi_2$$

Singular perturbation:

$$\xi_1' = r_1(\xi_1,\xi_2) \qquad\qquad 0 = r_1(\xi_1,\xi_2)$$

Generic procedure

1. Transform original state space into a state space better revealing important process dynamics

$$x - x^* = Uz$$

2. Decomposition into two complementary subspaces

$$Uz = U_1 z_1 + U_2 z_2, \qquad U = [U_1, U_2]$$

Substitution into original DAE system and decomposition yields

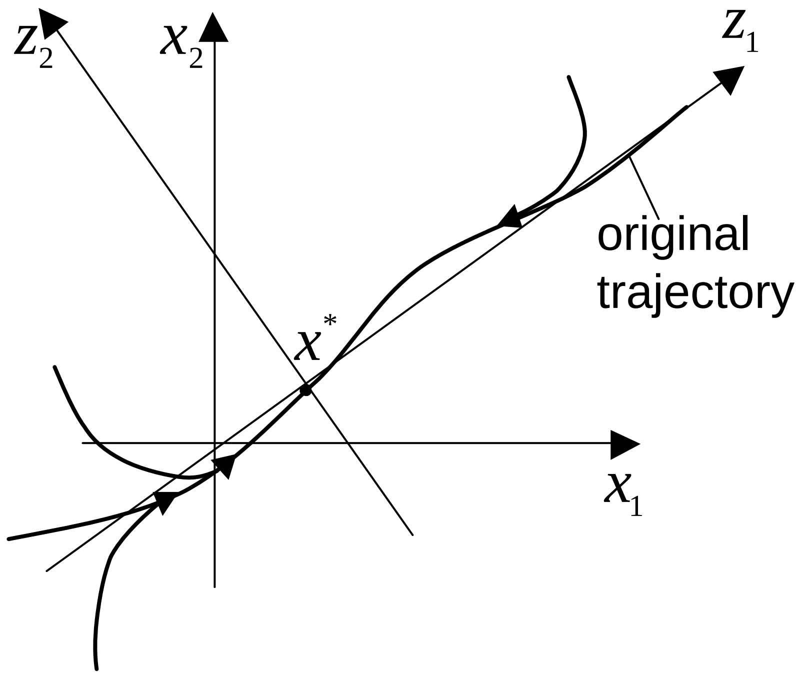
$$\dot{z}_1 = U_1^T f(x^* + U_1 z_1 + U_2 z_2, y, u)$$

$$\dot{z}_2 = U_2^T f(x^* + U_1 z_1 + U_2 z_2, y, u)$$

$$z_1(0) = U_1^T (x_0 - x^*)$$

$$z_2(0) = U_2^T (x_0 - x^*)$$

$$0 = g(x^* + U_1 z_1 + U_2 z_2, y, u)$$



Model reduction by projection (II)

3. Deduction of a reduced model

a) Truncation $(z_2 = 0)$

$$\dot{z}_1 = U_1^T f(x^* + U_1 z_1, y, u)$$
$$z_1(0) = U_1^T (x_0 - x^*)$$
$$0 = g(x^* + U_1 z_1, y, u)$$

- lower number of equations and variables than original model
- not steady-state accurate

b) Residualization $(\dot{z}_2 = 0)$

$$\dot{z}_1 = U_1^T f(x^* + U_1 z_1 + U_2 z_2, y, u)$$
$$0 = U_2^T f(x^* + U_1 z_1 + U_2 z_2, y, u)$$
$$z_1(0) = U_1^T (x_0 - x^*)$$
$$0 = g(x^* + U_1 z_1 + U_2 z_2, y, u)$$

- same size as original model, but less differential and more algebraic equations and variables
- steady-state accurate

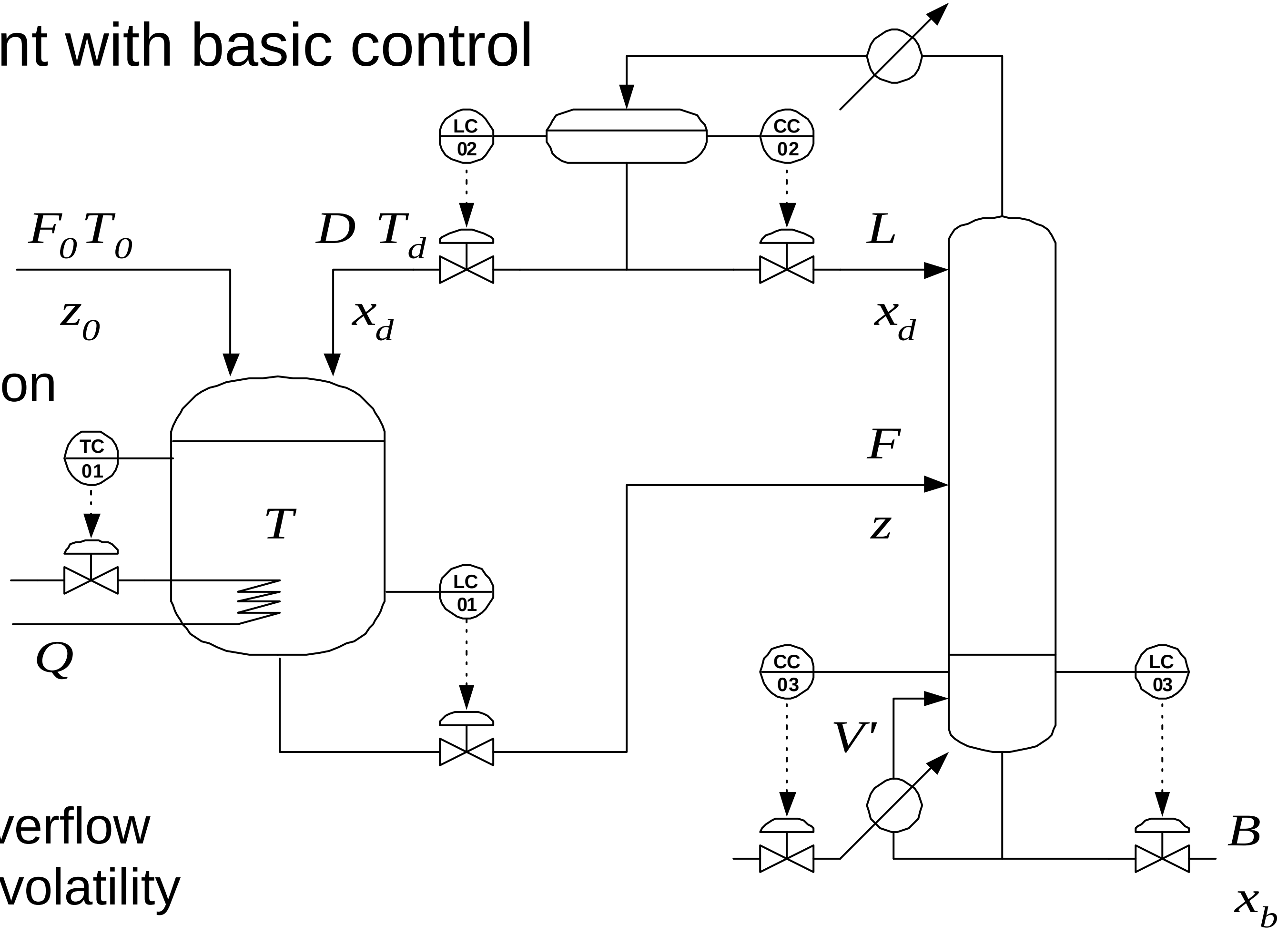
Model reduction by projection

- Problem
  - How to compute this transformation matrix?
- Options
  - Physical based lumping
  - Gramian based input output balancing transformations
  - Proper orthogonal decomposition
- Properties
  - Reduces the number of differential equations
    - Linear control problems are reduced with n-cubed
  - Increases the complexity of the model
    - Effort numerical integration will not be reduced if structure was exploited by the solver

Dynamics of plant with basic control

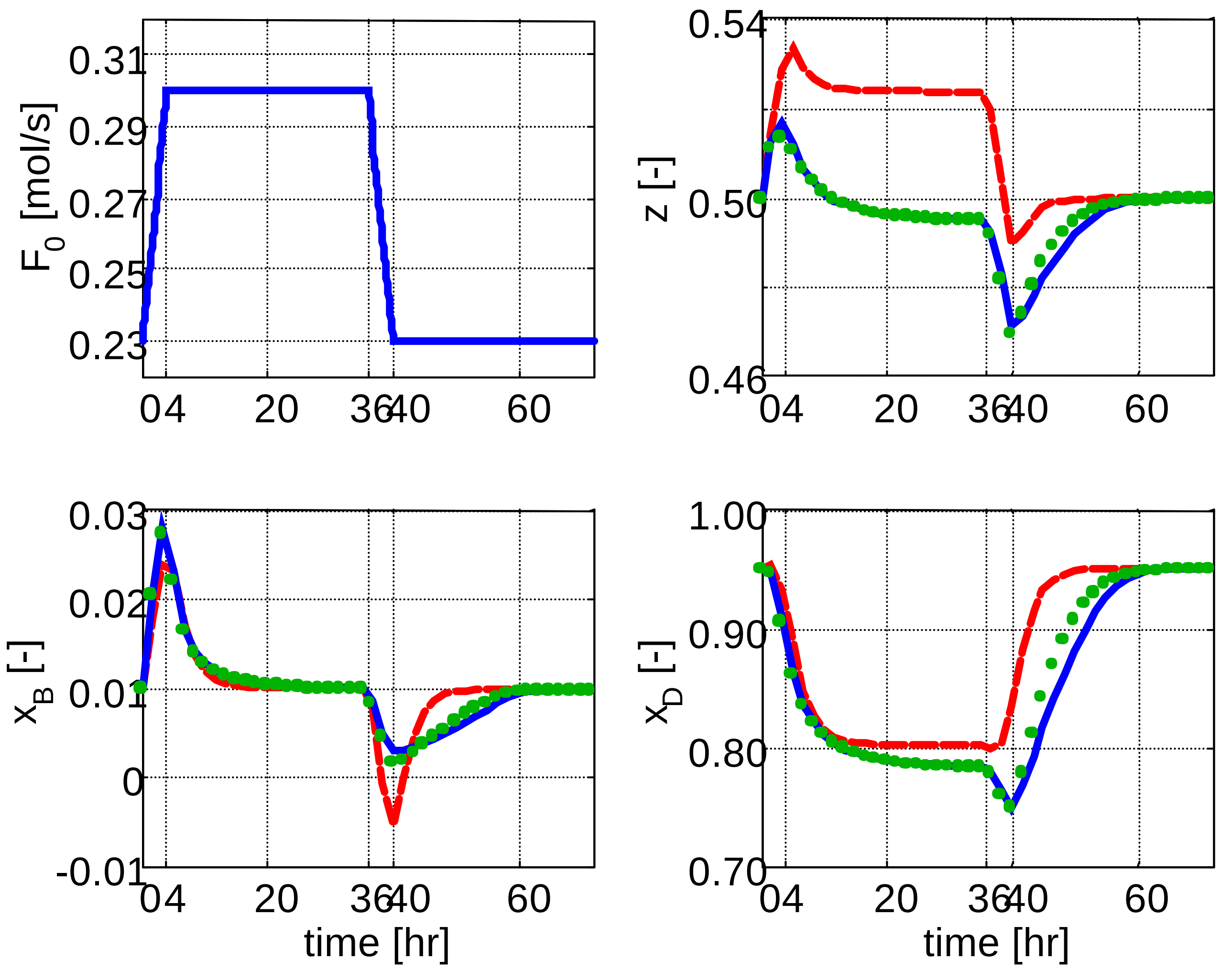
Reactor:
- exothermic reaction

$$A \rightarrow B$$



Column:
- constant molar overflow
- constant relative volatility
- 41 trays

Model reduction by Gramian based truncation



legend: original 45th order, linearized 45th order, reduced 4th order.

Proper orthogonal decomposition (POD)

Starting point: Representative trajectory for given x_0 and $u(t)$

1. Uniformly sample trajectory: *snapshot matrix* $X = [\Delta x(t_1), \Delta x(t_2), \ldots, \Delta x(t_p)]$

   with $x(t_k) - x^* = \Delta x(t_k)$

2. Singular value decomposition of X yields basis $U = [d_1, d_2, \ldots d_p]$

3. a) Select $p_1 << p$ *left singular* vectors of X

   $\Rightarrow$ associated with largest singular values $\Rightarrow$ capture dominant dynamics

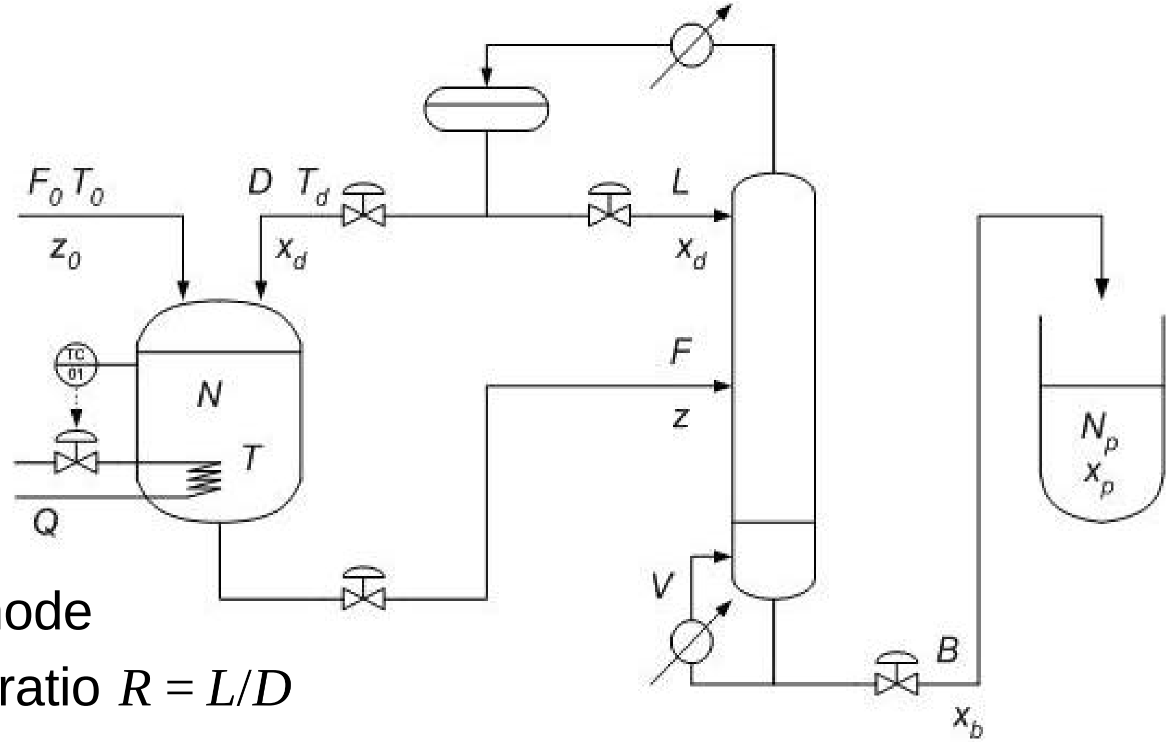
   $\Rightarrow$ corresponds to *truncation*

   b) Use all p singular vectors of X as basis

   $\Rightarrow$ can apply *residualization*

Case study optimization

Test plant



- Operated in semi-batch mode
- degree of freedom: reflux ratio $R = L/D$
- objective: minimize operation time t_f
- endpoint constraints
  - fixed amount of product $N_p(t_f)$ = 2000 mol
  - product composition $x_p(t_f)$ = 0.01
  - path constraint
  - reactor hold-up 350 mol <= N(t) <= 600 mol

Solution with truncated model (I)

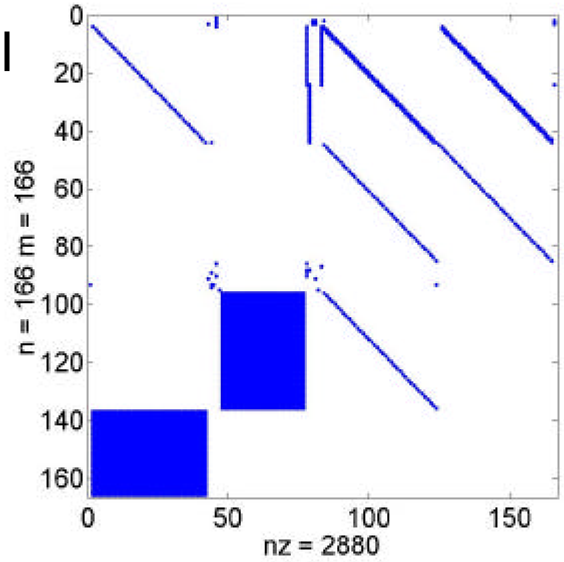
- Apply projection and truncation to column model
- Original column model: 41 trays = states
- 5 levels of reduction:

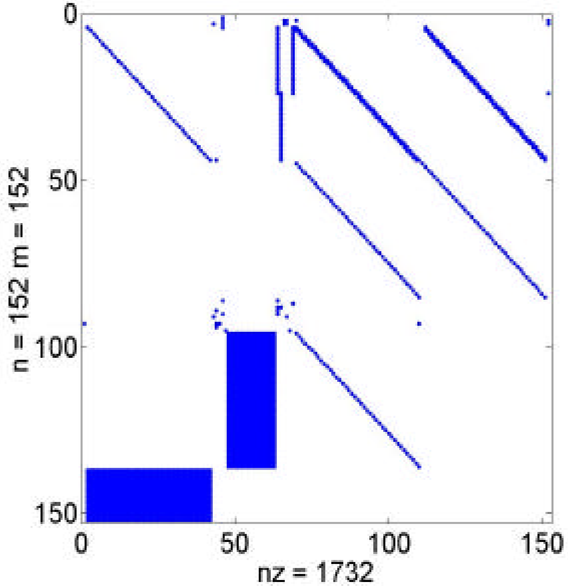
  $n_z = \{30, 20, 18, 16, 8\}$

	model order	ite-rations	inte-grations	obj. fun. value	CPU time [s]
nominal	41	31	73	8918.618	169.7
truncation	30	31	73	8918.622	758.1
	20	30	68	8921.933	562.4
	18	27	54	8889.999	397.6
	16	25	64	8958.987	317.5
	8	*problem infeasible*			

- Projection partly destroys sparsity

  $\Rightarrow$ strongly increased CPU time
- Projection deteriorates optimality



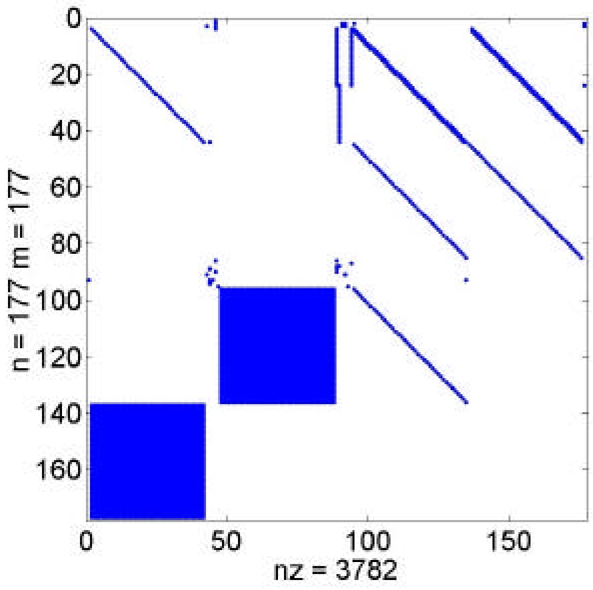


Solution with residualized model

- Apply projection and residualization to column model
- Original column model: 41 trays = states
- 3 levels of reduction:

  $n_z = \{30, 16, 8\}$

	model order	ite-rations	inte-grations	obj. fun. value	CPU time [s]
nominal	41	31	73	8918.618	169.7
residu-alization	30	31	73	8918.618	975.6
	16	32	77	8918.614	1083.2
	8	31	74	8916.406	1025.8



- Solution almost identical to nominal case
- Matrix fill-up independent of reduction level

  $\Rightarrow$ CPU time in the same order of magnitude, but much higher as nominal

Nonlinear Estimation I

- Problem
  - Need state to initialize model
  - Given measured data produce state-estimate
- Solution
  - Least squares horizon estimation
  - LTV approximation instead of true nonlinear
  - Single step LTV gives Extended Kalman Filter (EKF)
- Features:
  - Multi-rate measurements
  - Constraints on process variables
  - Delayed measurements
  - Primitive line-search

Nonlinear Estimation II

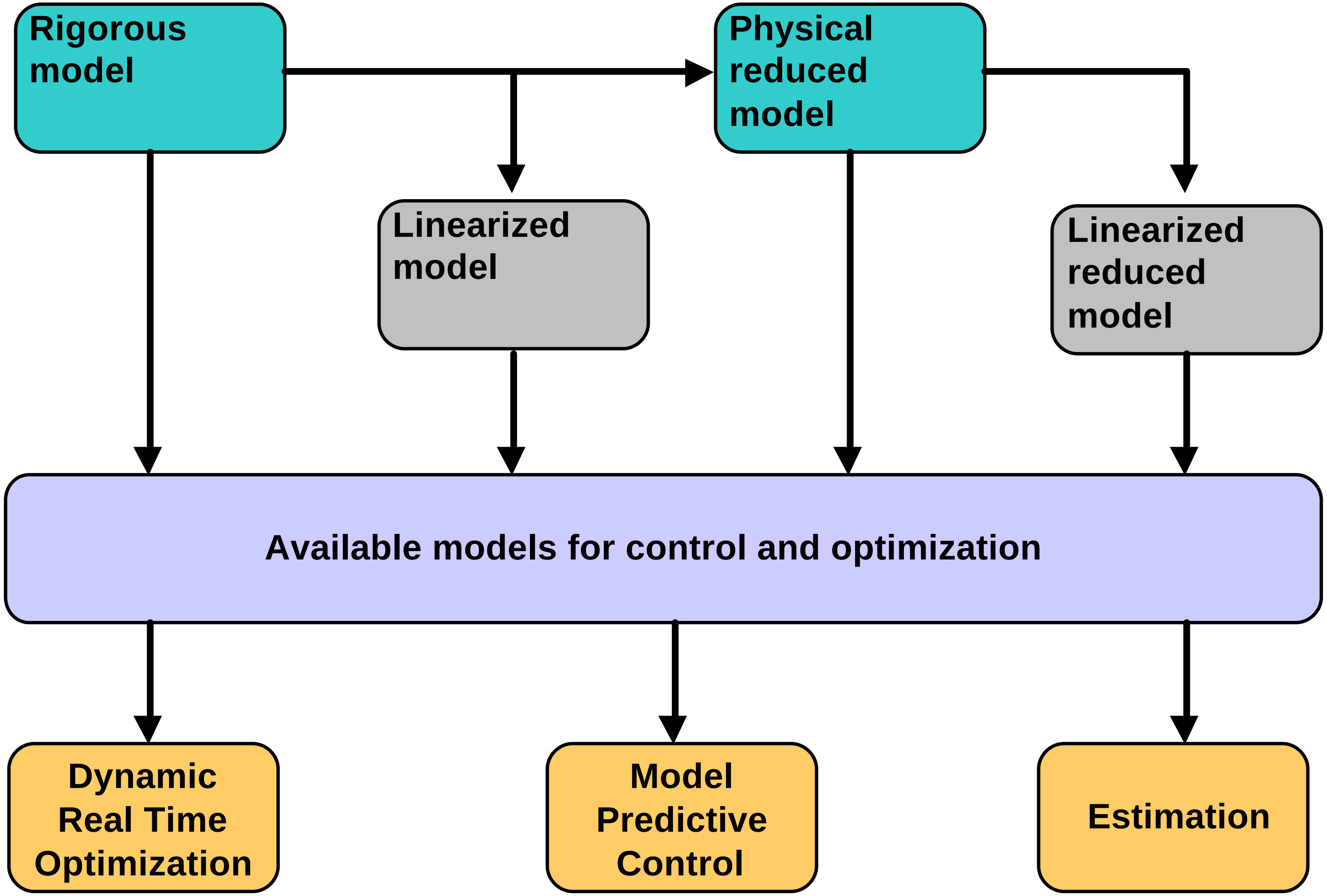
- Problem
  - Large number of parameters > nx+H*nw
  - Ill-conditioning of estimation problem
  - Tuning estimation function difficult
- Solution
  - Select only relevant input/output behaviour
  - Reduce number of differential variables
  - Uncertain feeds/energy flows to measured process variables
  - I/O balanced model-reduction
- Properties
  - Well conditioned small problem
  - Physical interpretation in dominant modes
  - Online feasible / reliable from certain number of states downwards

Model reduction for Estimation III

• Compute Jacobian of the model	$\dot{x} = f(x, y, u)$ $0 = g(x, y, u)$
• Derive linear model	$\Delta\dot{x} = A\Delta x + B\Delta u$ $\Delta y = C\Delta x + D\Delta u$
• First reduction linear model with fixed projection *(e.g. remove connectivity)*	$\Delta\dot{z} = \tilde{A}\Delta z + \tilde{B}\Delta u$ $\Delta y = \tilde{C}\Delta z + D\Delta u$
• Second reduction on reduced linear model by balanced truncation (online)	$\Delta\dot{z}_b = \hat{A}\Delta z_b + \hat{B}\Delta u$ $\Delta y = \hat{C}\Delta z_b + D\Delta u$

Significant computational savings obtained due to n^3 effect in control computations

Available models for control and optimization



Discussion

- Is it possible to reduce the model while retaining structure?

- Can one reduce the number of equation significantly?

- Can the application aspect be directly considered in the reduction procedure?

Conclusions

- Model synthesis: systematic approach needed

- Model reduction for ChE DAE systems: mixed results
  Reducing number of equations helps better than shifting the balance between ODE's and AE's in DAE problems.
  If algorithms exploit sparsity, order reduction is less effective.

- Modelling and model complexity reduction for integrated d-optimisation & control largely open
  Key issues:
  - *combination of fundamental and empirical model components*
  - *physical based lumping (species, phases, reactions)*
  - *model complexity reduction*
  - *real time adaptation of structure of reduced models*
  - *consistency of reduced models for various tasks*
  - *closed loop model validation*

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