Reduced chemical kinetics for combustion and ignition

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Overview

- introduction
- ILDM
- problems and solutions
  - numerical calculation
  - manifolds of stationary states higher order
  - reduced ignition chemistry
  - implementations of reduced chemistry
- summary

Simulation of combustion processes

combustion chemistry

complete description by elementary reactions

--> detailled mechanisms

flow field

conservation equations for every chemical species

--> small mechanisms

reduced mechanisms

accuracy of detailled mechanisms

small number of reaction progress variables

Reduction of detailled reaction mechanisms

conventional methods

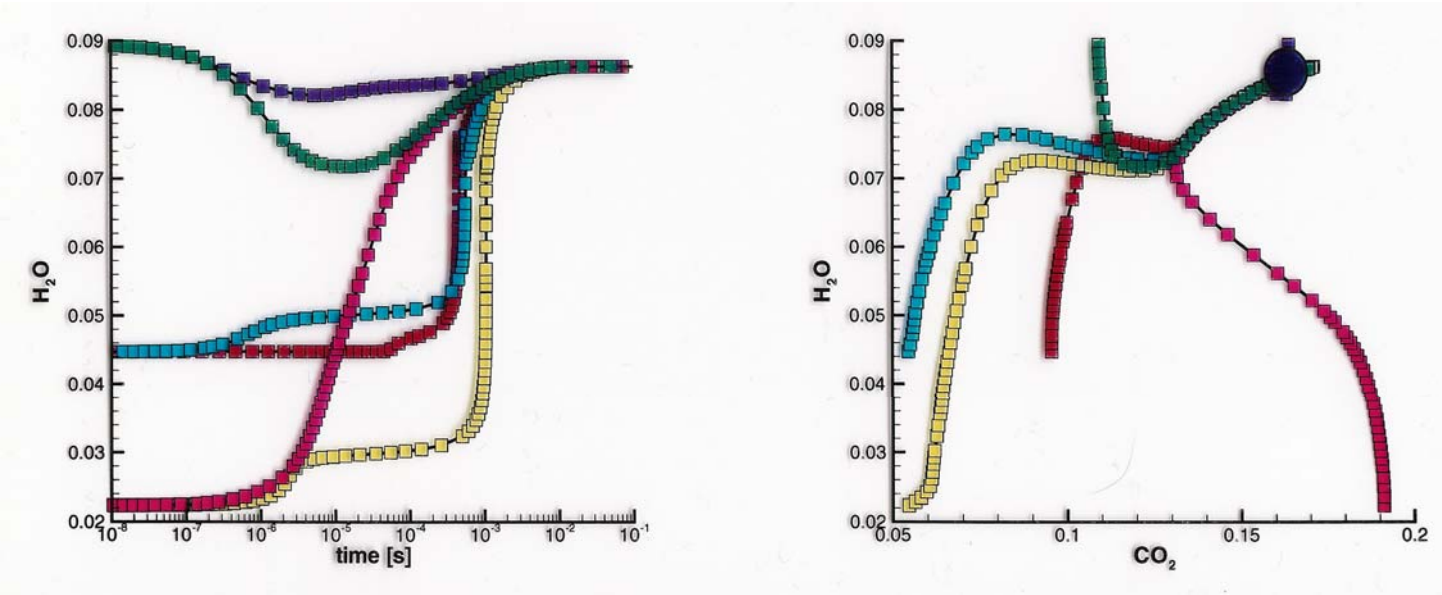
assumption of *** partial equilibrium for reactions**
*** stationary state of species**

disadvantage: physical motivation of assumptions restrict the reduced mechanism to specified conditions (e.g. high temperatures, lean conditions)

ILDM-method

- **reduction to the rate limiting slow part of the mechanism**
- **mathematical/numerical method**
- **only input: number of reaction progress variables**

Homogeneous reactor in state space

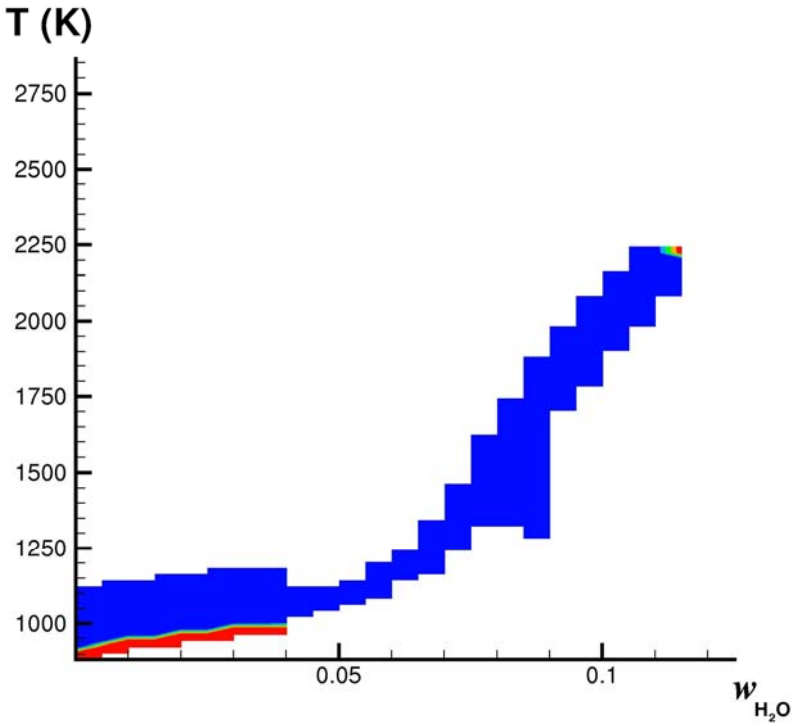


fast reaction to **Intrinsic Low-Dimensional Manifolds (ILDM)** in state space

Idea: use ILDM as a basis for a mechanism reduction method (Maas, Pope 1992)

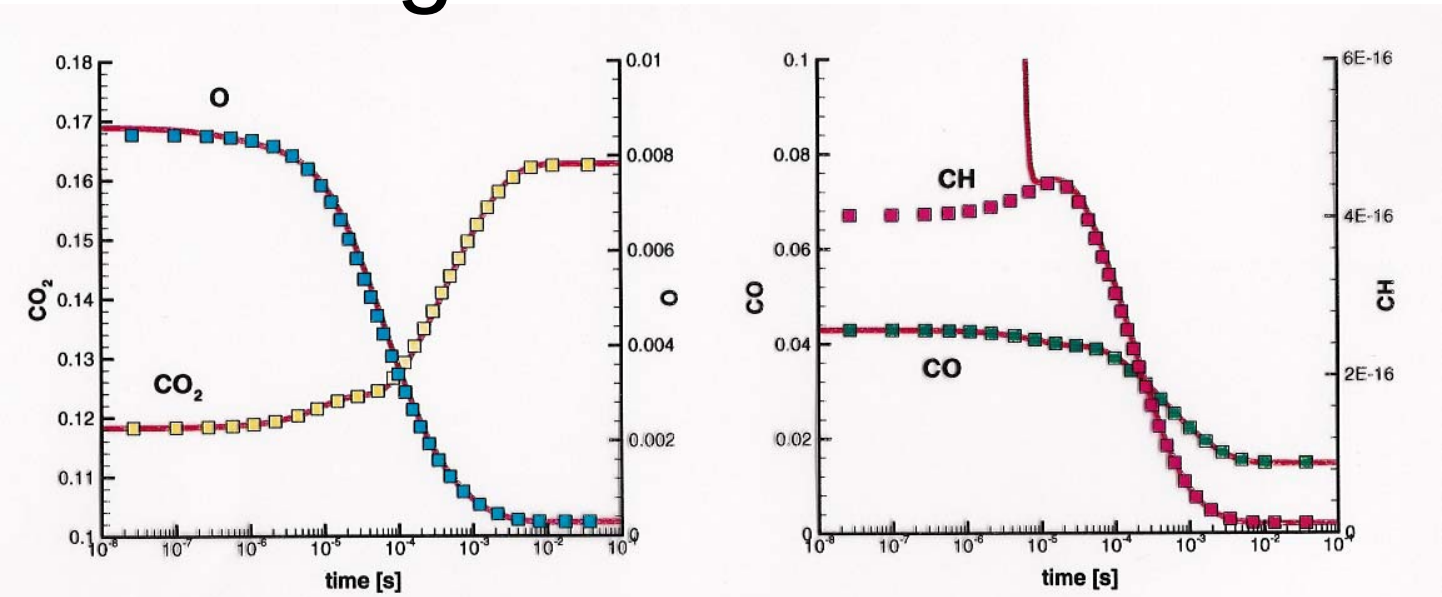
---> identification of rate limiting part of reaction mechanism

Tabulation of ILDM



- calculation of ILDM is computationally expensive
- solution: tabulation and use of fast table look-up instead of slow calculation

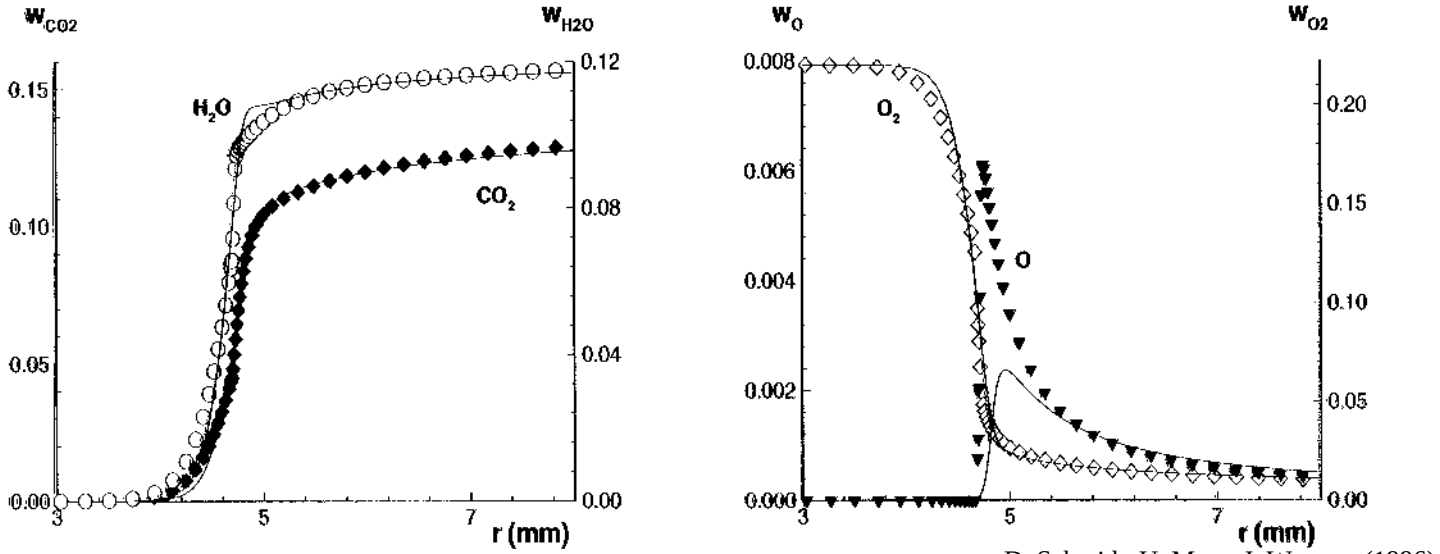
Application: homogeneous reaction



- **initial conditions: partially burnt stoichiometric mixture dodecane-air (temperature of unburnt mixture 300 K, 1 bar)**
- **lines: detailed mechanism; symbols: ILDM**
- **2 reaction progress variables CO_2 and H_2O**
- **very good comparison both for main species CO_2 and CO as for the radicals O and CH**

---> mechanism reduction with ILDM-method is highly accurate

Application: flame 2d-ILDM



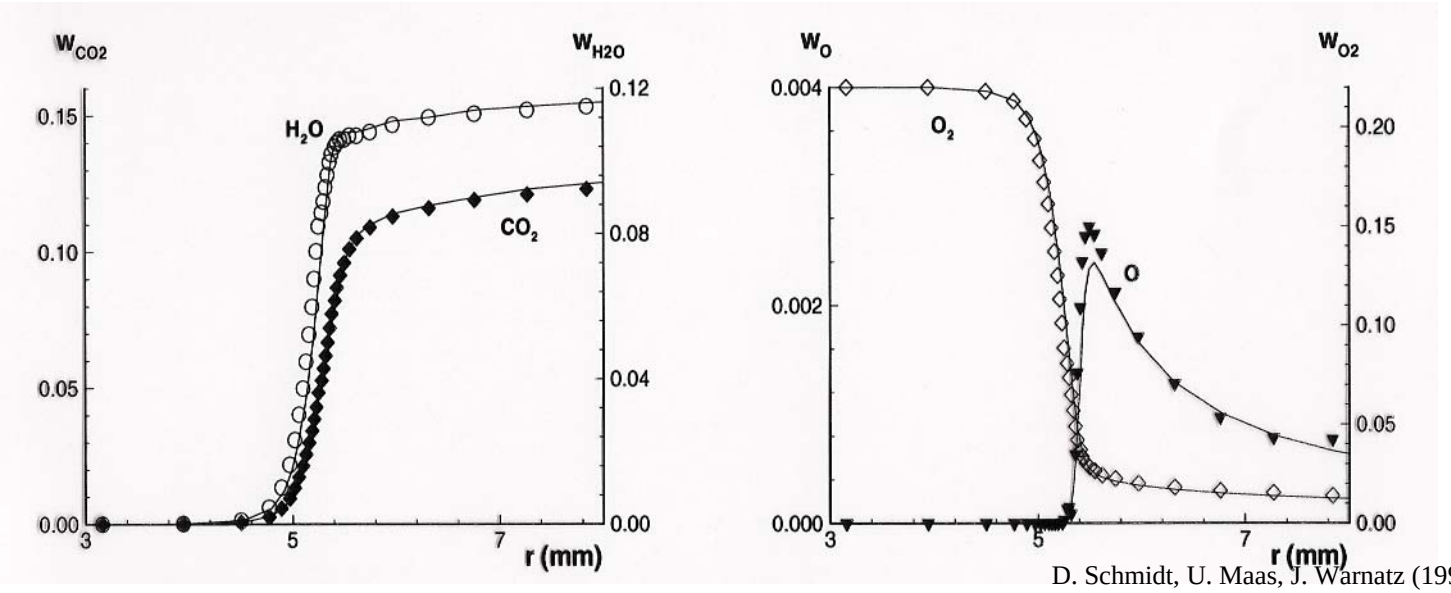
D. Schmidt, U. Maas, J. Warnatz (1996)

- **laminar premixed flame methane-air (stoichiometric, 300 K, 1 bar)**
- **lines: detailed mechanism; symbols: ILDM**
- **2 reaction progress variables CO_2 and H_2O**
- **good comparison for main species CO_2, H_2O and O_2**
- **deviations with O-atoms**

---> influence of diffusion on the relaxation of fast chemical time scales

---> improvement by additional reaction progress variable O_2

Application: flame 3d-ILDM

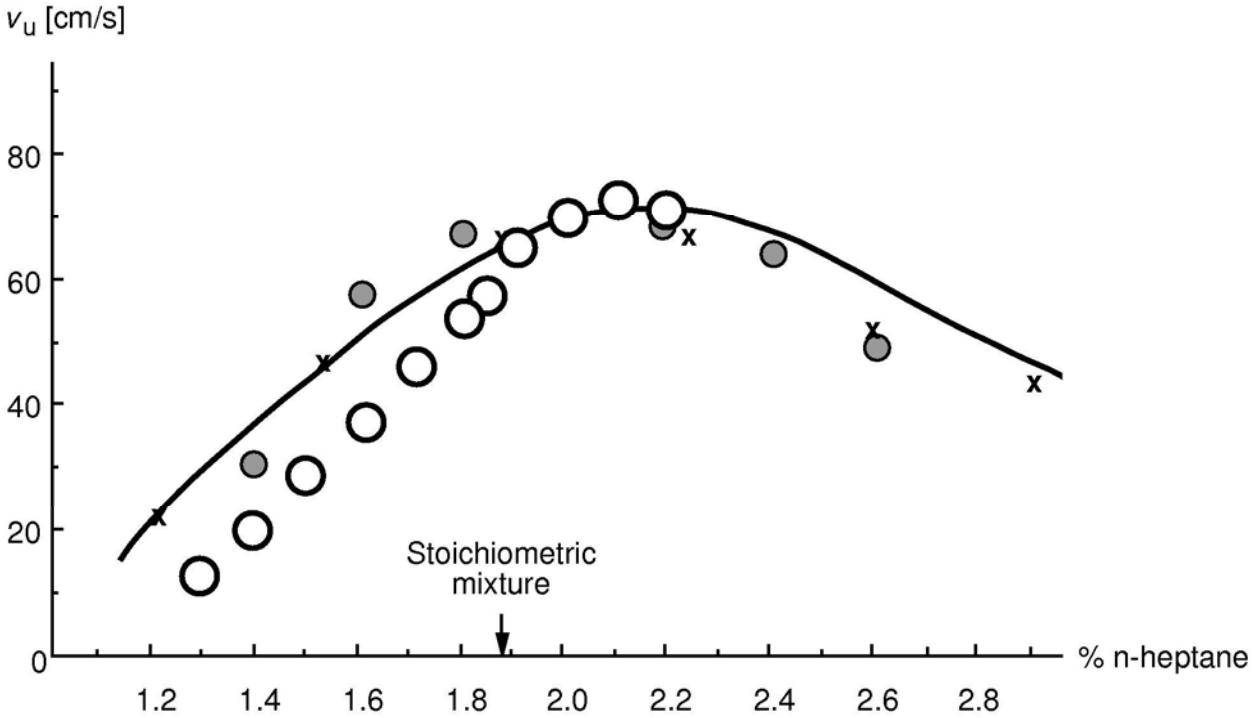


D. Schmidt, U. Maas, J. Warnatz (1996)

- **laminar premixed flame methane-air (stoichiometric, 300 K, 1 bar)**
- **lines: detailed mechanism; symbols: ILDM**
- **3 reaction progress variables CO_2, H_2O and O_2**
- **very good comparison for main species CO_2, H_2O and O_2**
- **small error for O-atoms**

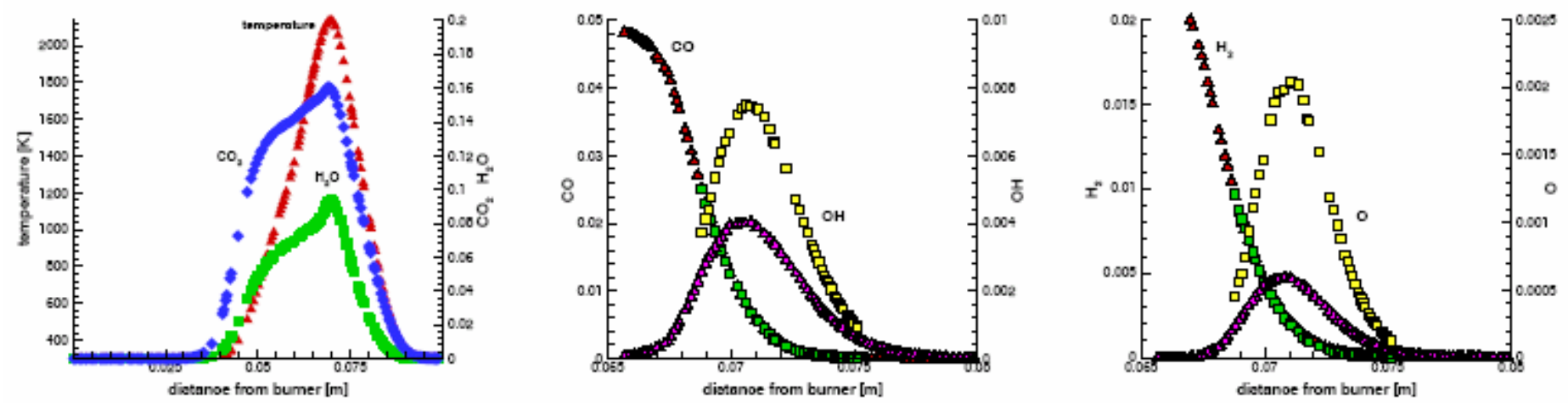
---> 3 reaction progress variables are sufficient for laminar premixed flames

Application: flame velocities



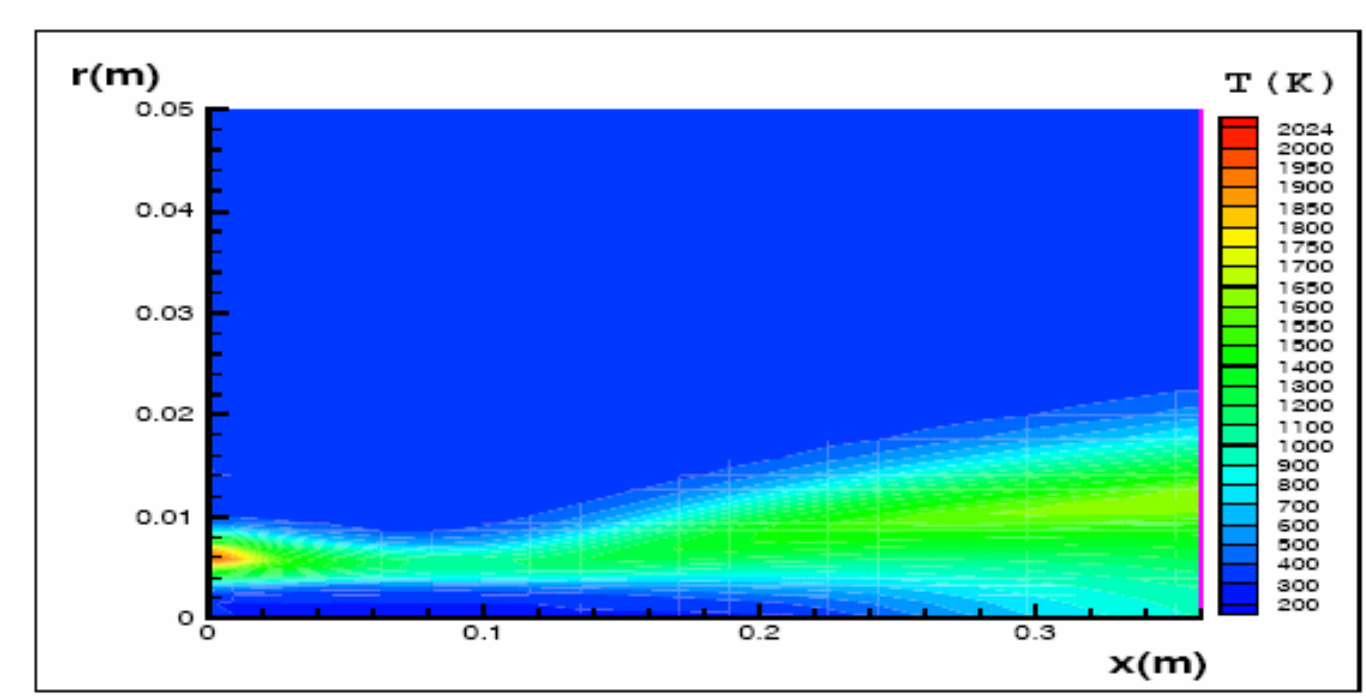
- laminar premixed flame heptane-air (800 K, 80 bar)
- lines: detailed mechanism; detailed transport
- white symbols: ILDM; Le=1
- filled symbols: measurements

Application: Non-premixed flame



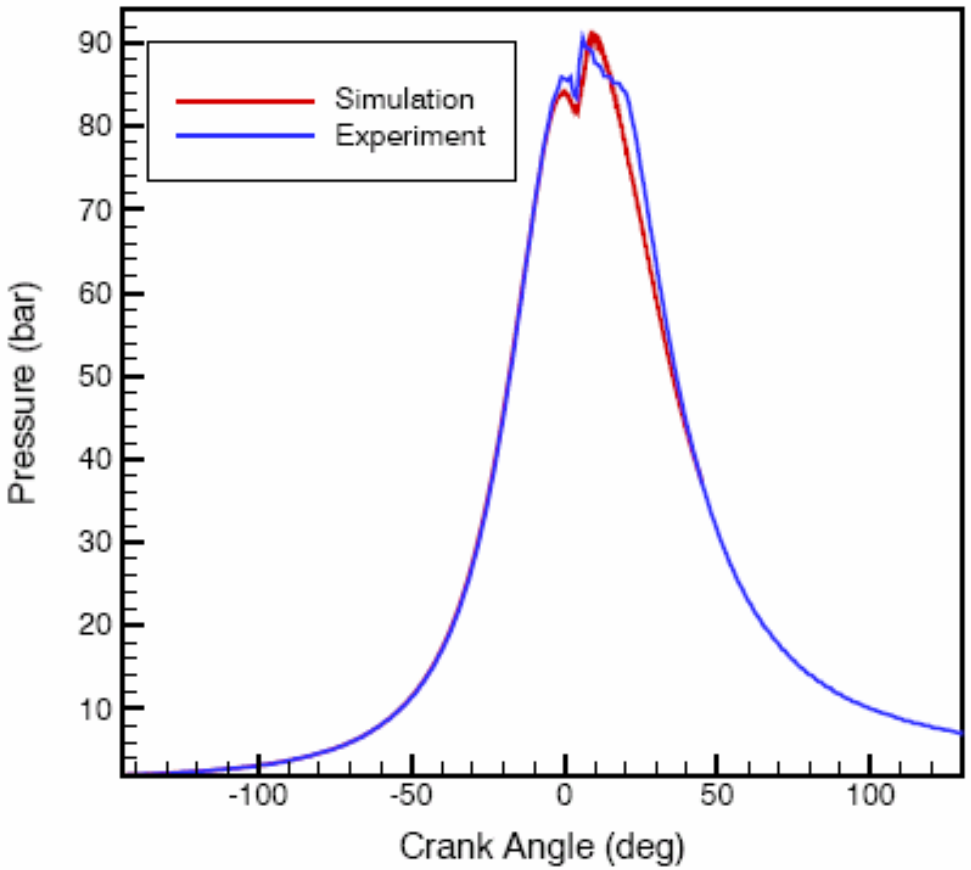
- **laminar non-premixed flame heptane-air (stoichiometric, 300 K, 1 bar)**
- **2 reaction progress variables CO_2, H_2O (temperature)**
- **very good comparison for main species CO_2, H_2O and O_2**
- **good comparison for minor species**

Application: turbulent jet-flame



- **non-premixed flame methane-air**
- **turulence-chemistry interaction: PDF, Monte-Carlo-method**
- **2 reaction progress variables CO_2, H_2O, temperature**

Application: Diesel engine



Correa (2000)

- Turbulence-chemistry-interaction: Presumed PDFs
- 3-dimensional ILDM table (temperature, CO_2, H_2O)

Is ILDM the perfect method for mechanism reduction?

- All slides look fine!
- All relevant applications have been done!
- Where is the problem?

There still exist major problems!

- manifold
  - numerical calculation often fails
  - bug in theory? Strange results in homogeneous reactions
  - existence only in the burnt region: Ignition chemistry is not available
- tabulation
  - needs too much space
- implementation
  - needs experts

Definition of the manifold

- Chemistry: $\dot{x} = S(x)$
- Local linearization $J = \frac{\partial S(x)}{\partial x}$
- Eigenvalue decomposition $J = E\Lambda\tilde{E} = \begin{pmatrix} E_s E_f \end{pmatrix} \begin{pmatrix} \Lambda_s & \\ & \Lambda_f \end{pmatrix} \begin{pmatrix} \tilde{E}_s \\ \tilde{E}_f \end{pmatrix}$
  - Order in fast and slow
- Definition of the manifold: $\tilde{E}_f(x)S(x) = 0$

Calculation of the manifold I

- Solution of algebraic equation system is difficult
  - nonlinearity and
  - stiffness of reaction mechanism
- Reason for stiffness:
  - thermodynamics
  - higher alcanes are extremly unstable at equilibrium temperatures
- Stiffness is increasing with growing numbers of C-atoms in fuels

Calculation of the manifold II

- Conversion of
  - algebraic equation system $\tilde{E}_f(x)S(x) = 0$
  - with parameters $P^T x = p$
  - into an ODE system $\dot{x} = S(x) + \tilde{E}_s(x)q$

    $\dot{q} = f(x, p)$
- Solution with standard stiff-stable ODE-solvers

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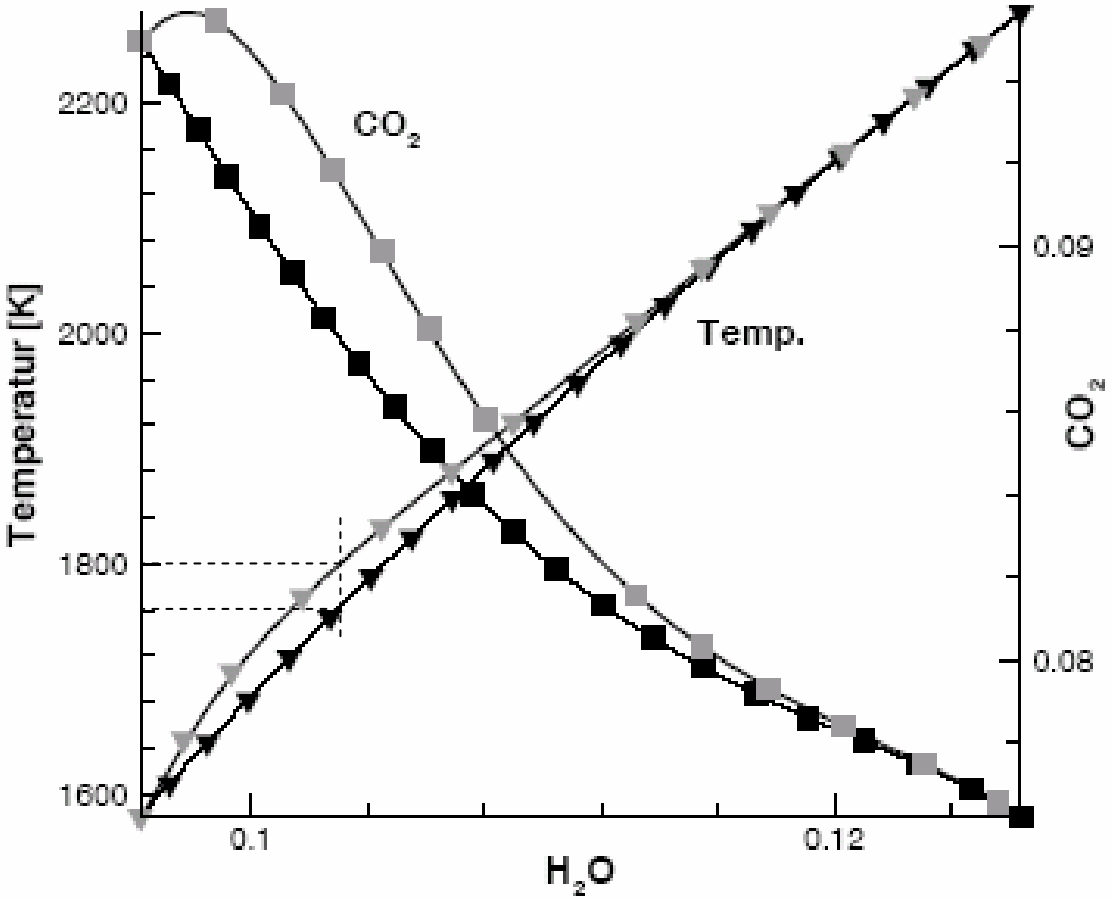
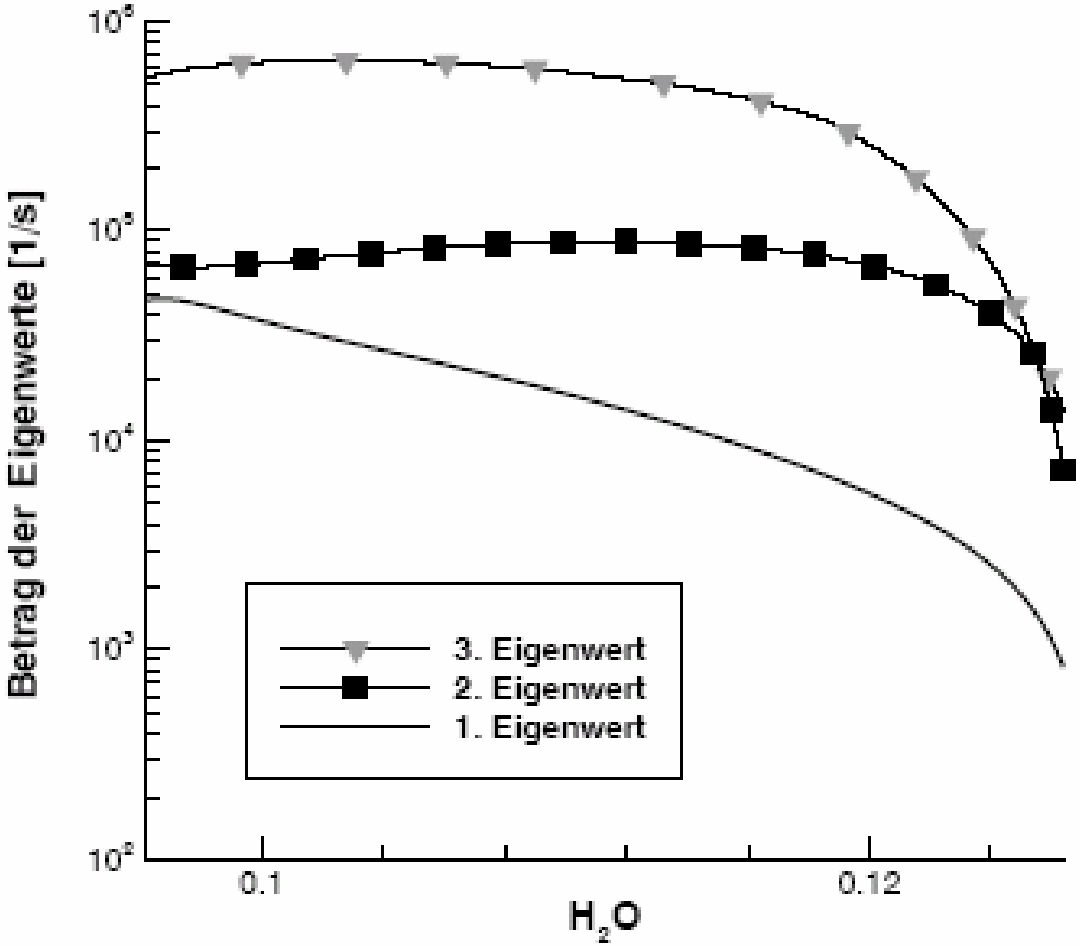
Bug in theory?

- Trajectories starting on the ILDM are leaving and deviating from the ILDM!
- Error of 40 K
- ILDM: black
- Trajectory: grey



Why there is a deviation?

- Small spectral gap
- definition of ILDM: Local non-linearity of reaction is neglected



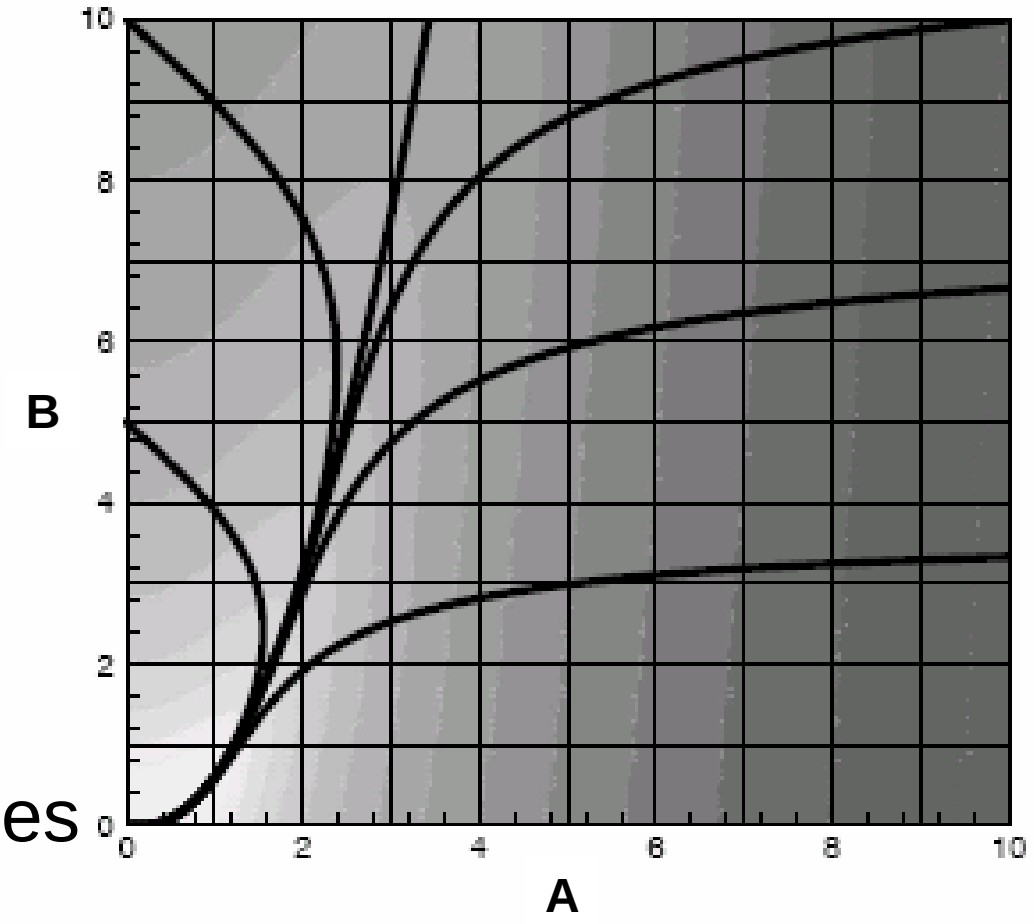
Investigation on a theoretical mechanism

- Reaction system

$$A + A \rightarrow C$$
$$B \rightarrow A$$

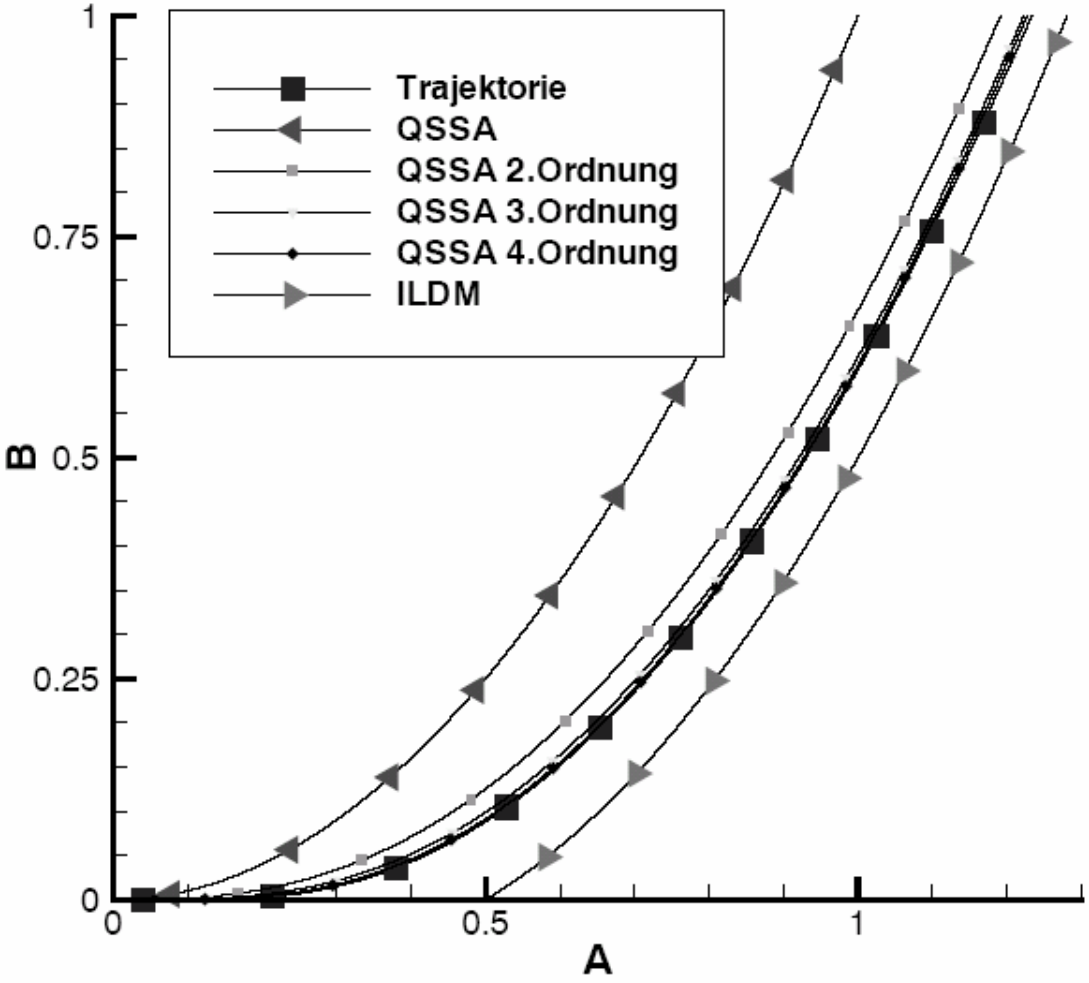
$$\begin{pmatrix} \dot{a} \\ \dot{b} \end{pmatrix} = \begin{pmatrix} -a^2 & +b \\ & -b \end{pmatrix}$$

- bundling trajectories

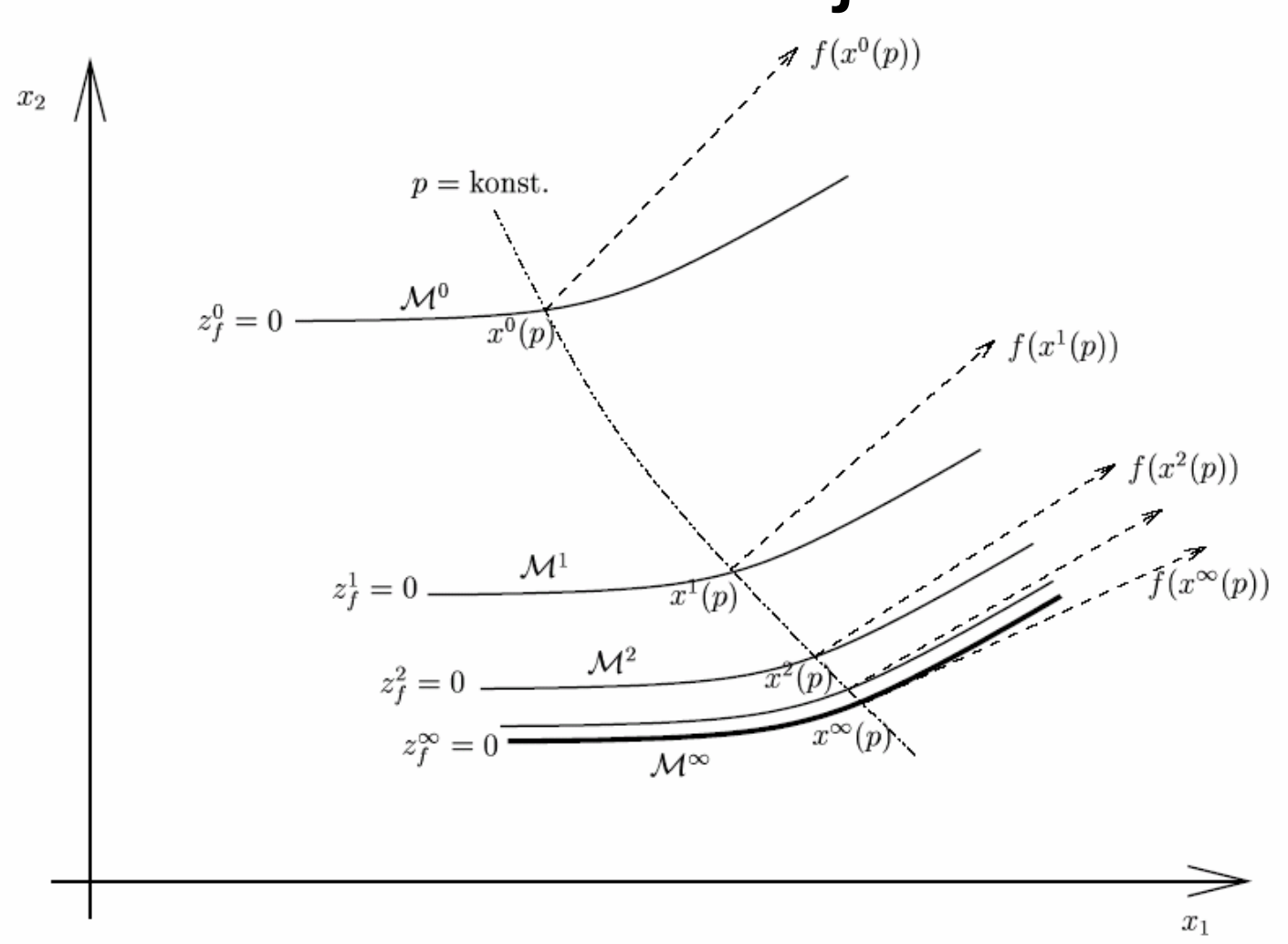


Series of manifolds of stationary states higher order

- ILDM is not a good approximation for the trajectory
- Series is converging to the trajectory



Proof: Series of manifolds of stationary states higher order is attractor for trajectories



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Reduced ignition chemistry

- Idea of ILDM: All chemical scales are in equilibrium
  - except the very slow ones
- Ignition: All chemical scales are frozen
  - except the very fast ones
- ILDM can not be used in ignition prediction!

Is a reduced ignition chemistry possible?

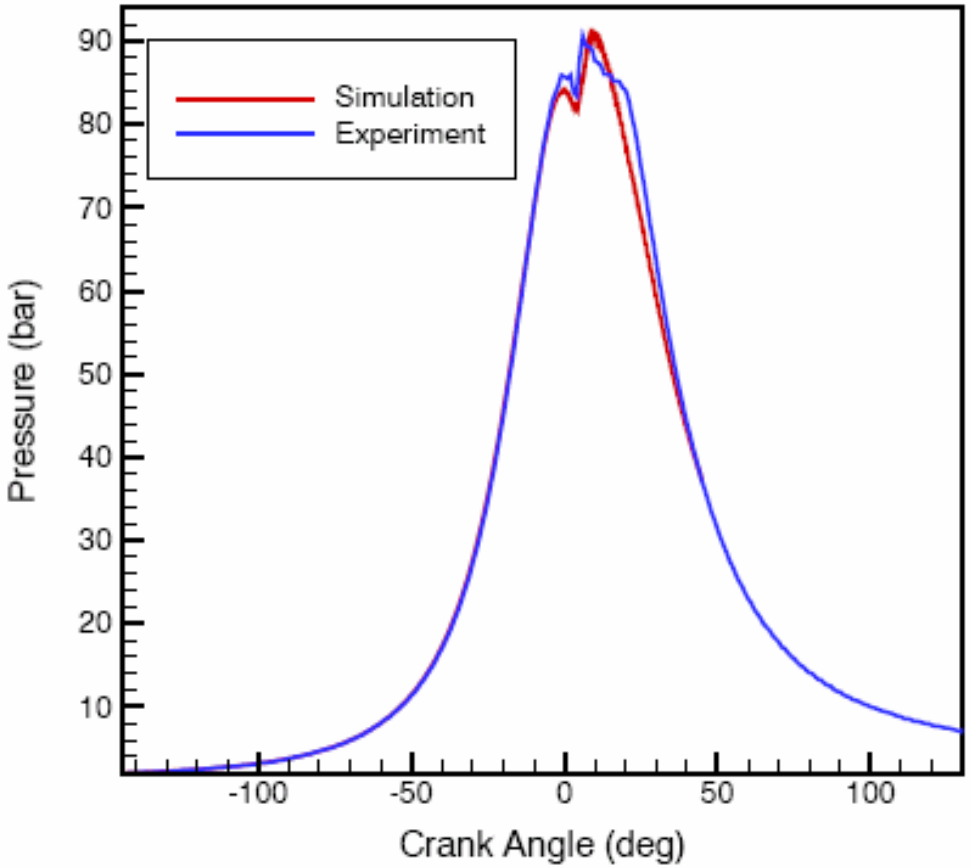
- Problem of dimensionality with ignition:
  - Equilibration of scales leads to a dimension reduction → no influence of initial conditions!
  - Ignition occurs with the dimension of the chemical state space (size of mechanism) →influence of initial conditions!

- No rigorous model with generally applicable reaction progress variables can be found for ignition

Reduced ignition chemistry

- But: In practical applications (e.g. CI engine) dimensionality of initial conditions is much smaller:
  - unreacted fuel-air mixture
  - variable temperature
  - variable pressure
- Idea: Use one reaction progress variable from trajectories
- Result: Table of reduced ignition chemistry with a few variables (mixture, temperature, pressure, one reaction progress variable)

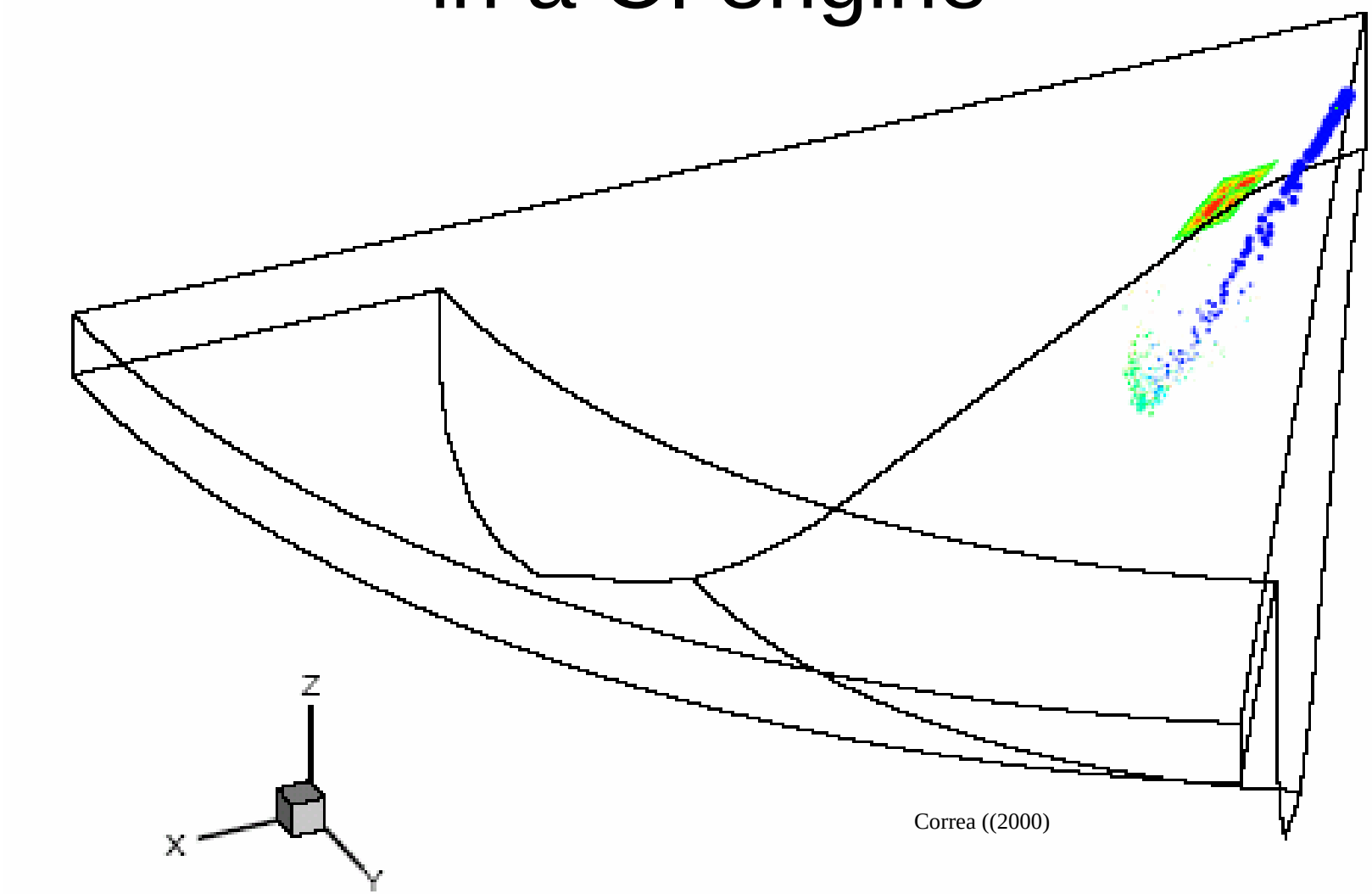
Applied Reduced ignition chemistry in a CI engine



Correa ((2000)

- Reduced ignition model + 3-dimensional ILDM (temp., CO_2, H_2O)
- Turbulence-chemistry-interaction: Presumed PDFs

Applied reduced ignition chemistry in a CI engine



Correa ((2000)

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Tabulation

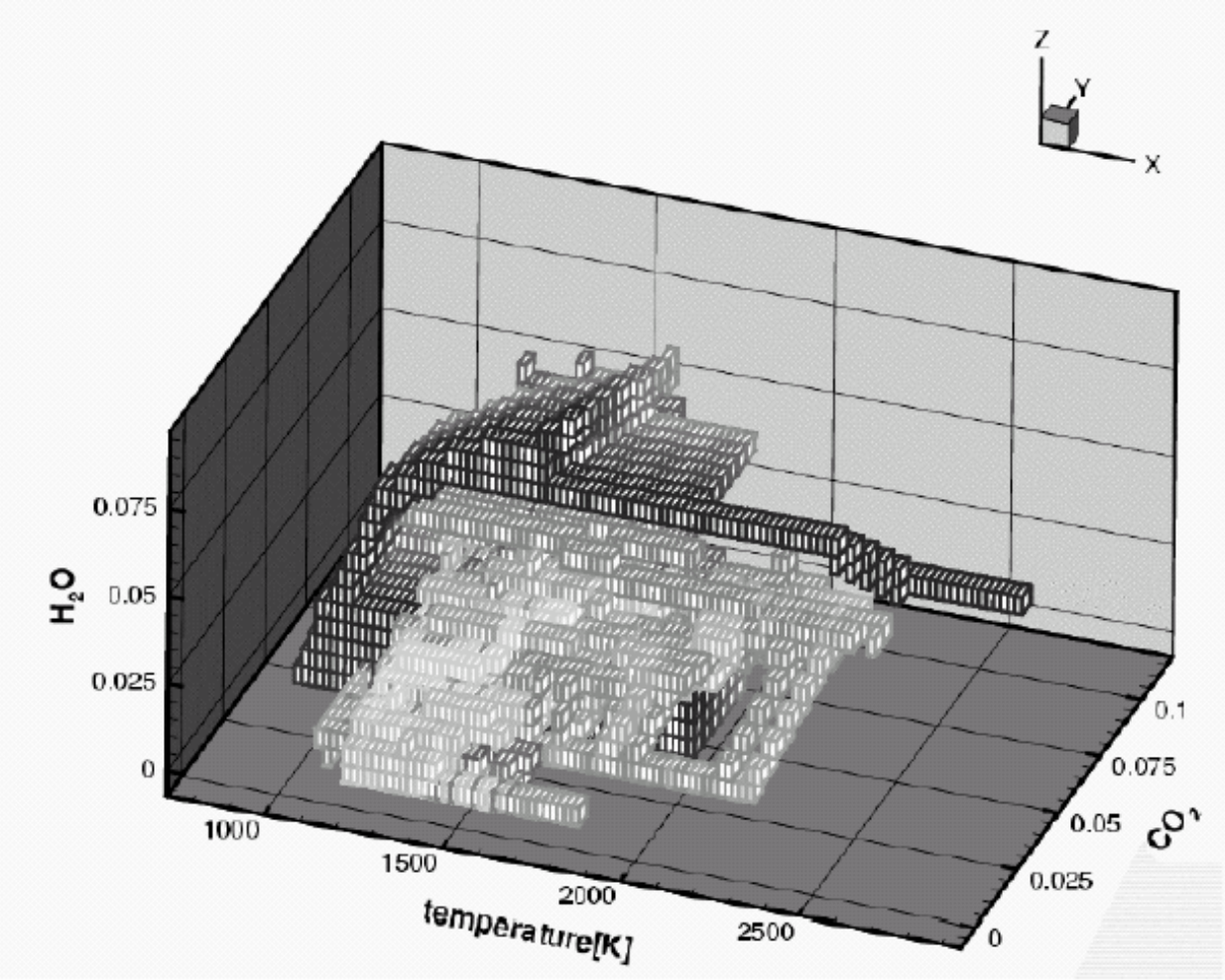
Dimensionality of reduced chemistry in a CI engine

- Temperature/enthalpy
- Pressure
- Mixture
  - Mixture fraction
  - More rigorous: 3 element mole fractions
- Reaction progress variables
  - 1: seems to work not too badly
  - More are better!

Result:

- 4 axis are the minimum
- In-situ tabulation is the only way to handle that big tables

Application of in-situ tabulation in a CI engine



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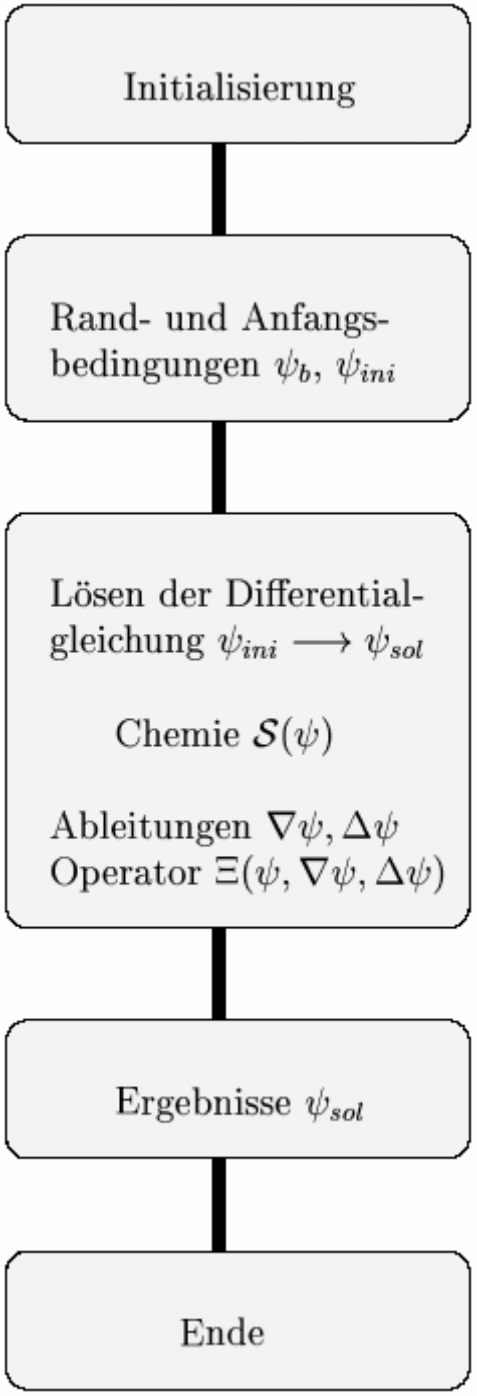
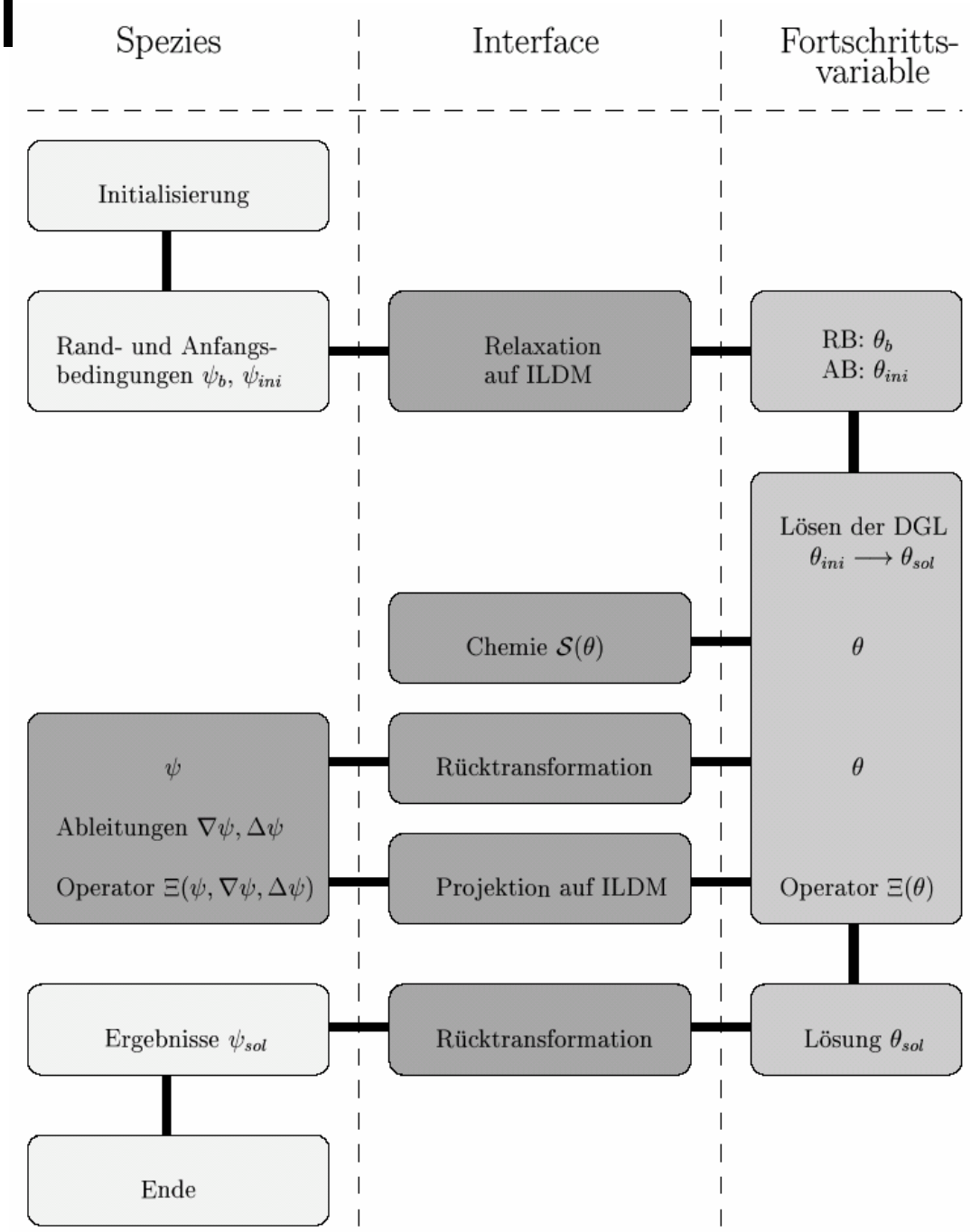
CFD-code

- How to implement tabulated manifold chemistry?
- Problems:
  - Reaction progress variables (RPV) are very different from species
  - Different RPV for ignition and combustion
  - Variable number of RPV → variable number of conservation equations



Conventional implementation of ILDM

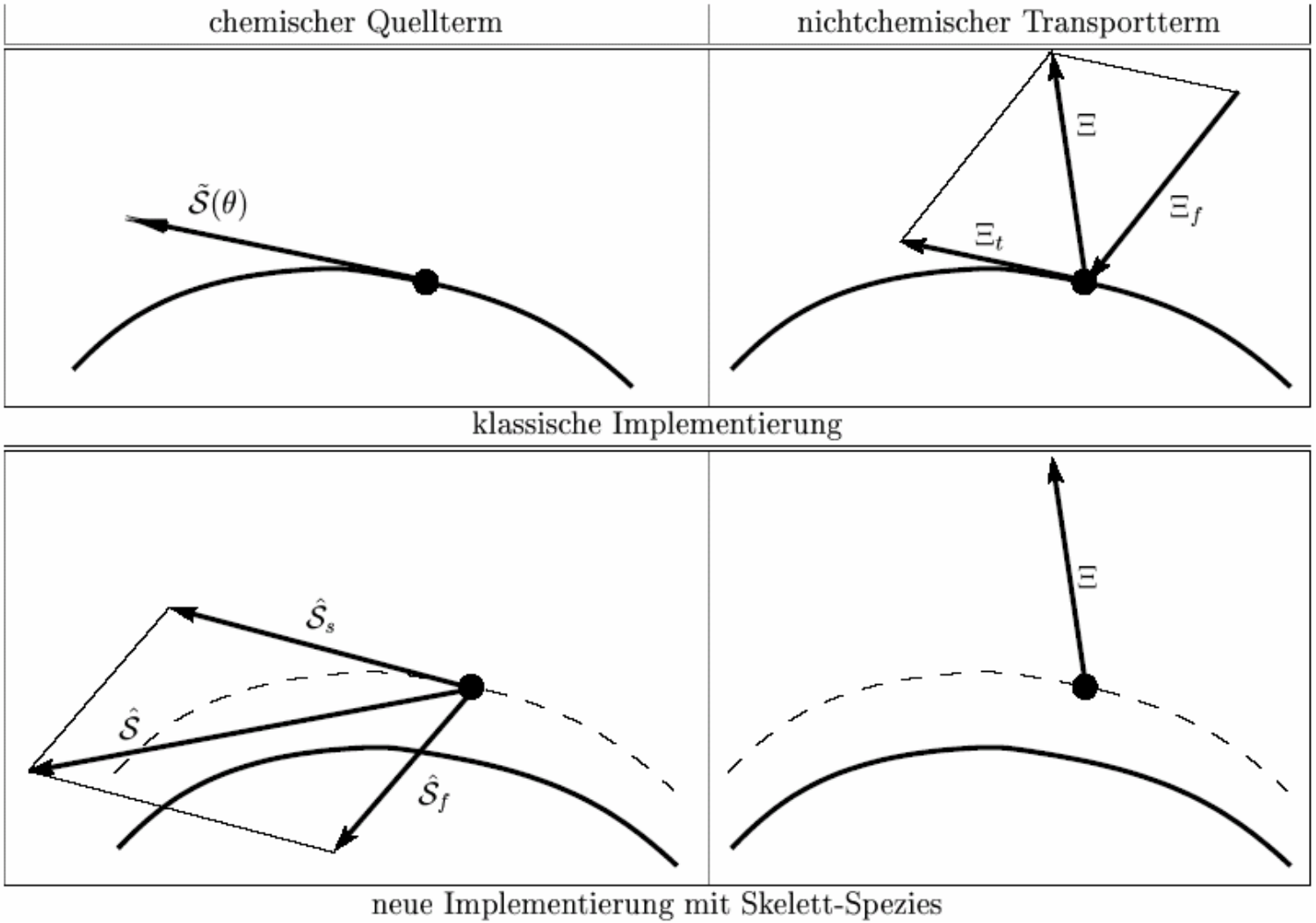
- Both RPV and species required
- Small reduction in space and computation time
- Diffent #RPV is a hard problem



Idea of sceleton mechanism implementation

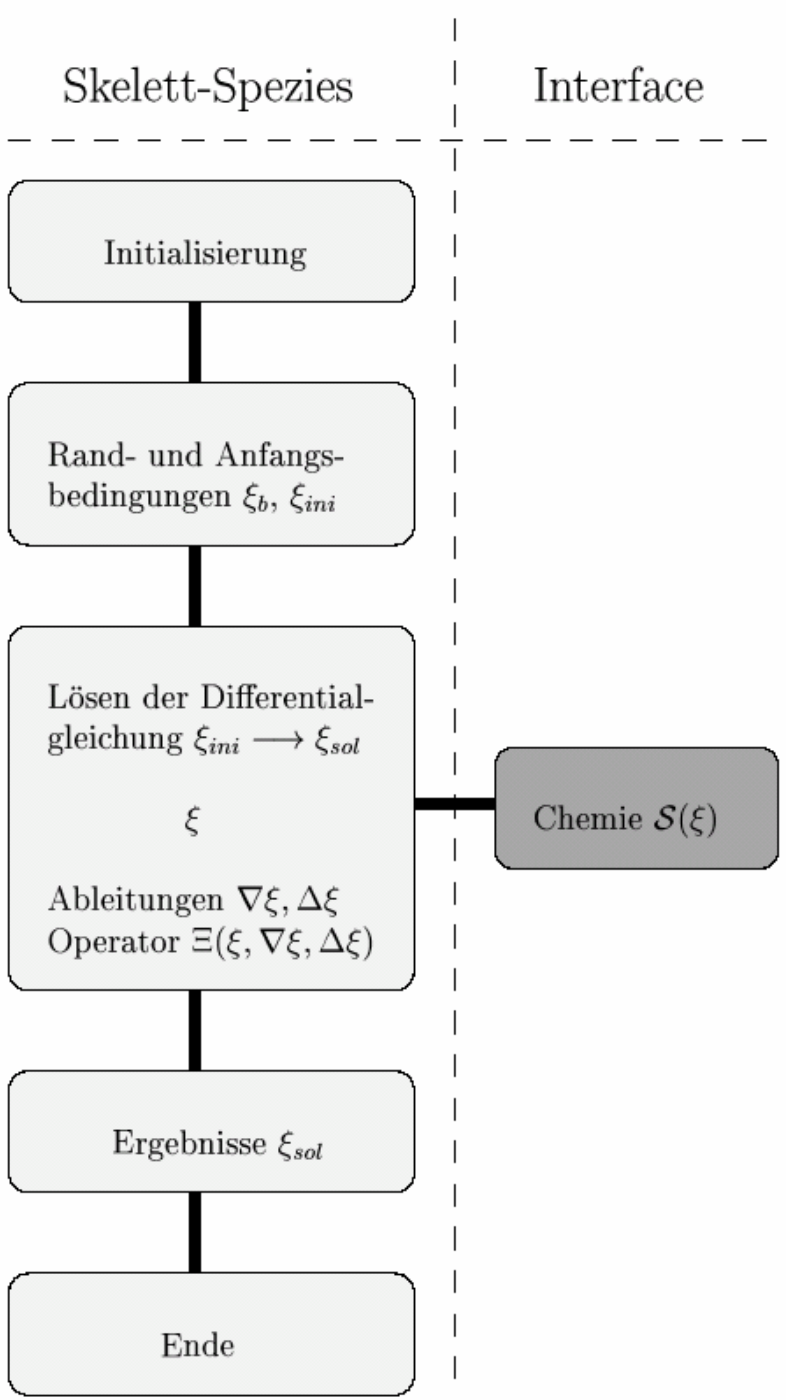
- Manifold chemistry should be usable like a skeleton mechanism
  - small number of species
  - Low stiffness
  - Details of the manifold (different models for ignition and combustion, variable dimension, …) should be hidden from the user
  - Physical interface layer

Idea of sceleton mechanism implementation



Sceleton mechanism implementation

- CFD-code is unchanged except the chemical source term
- Details of the manifold chemistry hidden in the chemical source term



Are there more problems?

- manifold
  - numerical calculation often fails
  - bug in theory? Strange results in homogeneous reactions
  - existence only in the burnt region: Ignition chemistry is not available
- tabulation
  - needs too much space
- implementation
  - needs experts

Summary: Reduced chemical kinetics for combustion and ignition

Combined Reduced Chemistry

- Manifold chemistry (ILDM, stationary states higher order) for the combustion/equilibration zone
- Reduced ignition chemistry
- In-situ tabulation
- Sceleton mechanism implementation