

Numerical simulations of large chemical kinetic systems



Leibniz Institute for
Tropospheric Research

using the - Atmospheric Chemistry Solver - an experimental environment for the simulation of large atmospheric multiphase mechanisms and detailed combustion systems

Willi Schimmel, Oswald Knoth

March 1, 2018

Leibniz Institute for Tropospheric Research, Department: Modelling of Atmospheric Processes

Outline

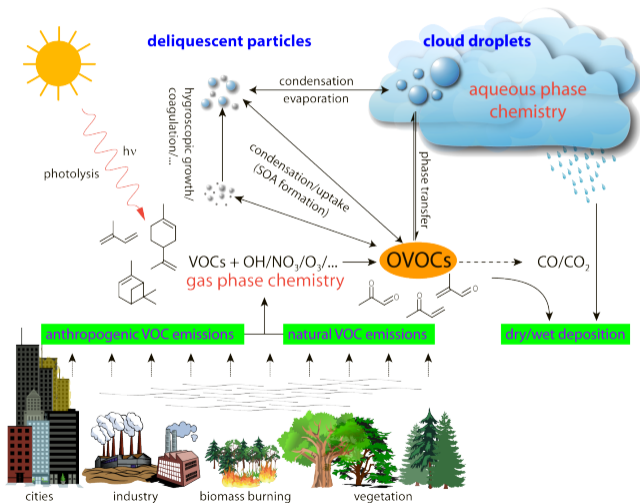
- ① Introduction and Motivation
- ② Model Description
- ③ Numerical Solver
- ④ Summary and Further Work

Introduction and Motivation

Practical applications of reaction kinetics

modelling of atmospheric chemical processes

- main actor for cleaning the atmosphere and precursor for new particle formation
- MCM** gas phase chemistry (Uni of Leeds, UK Met Office)
- CAPRAM** liquid phase chemistry (TROPOS)
- incorporate into higher dimensional CFD models
- improving efficiency is crucial



Practical applications of reaction kinetics

modelling of ignition and combustion

- modeling power stations, turbines, engines, rockets
- mechanism size depends on maximal number of hydrocarbons
- improving combustion of biodiesel fuels
- minimising emission rates
- main application for new numerical methods

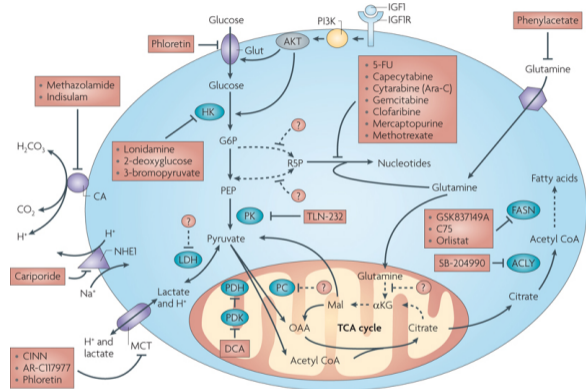


STS-28 Atlantis launch, source: nasa.gov

Practical applications of reaction kinetics

modelling biochemical processes within living organisms

- metabolic networks (e.g. medical drug decomposition in the body)
- modelling the cell cycle
- simulation of infection processes
- difficulties resulting from intrinsic multi-scale and stochastic nature of the biological processes

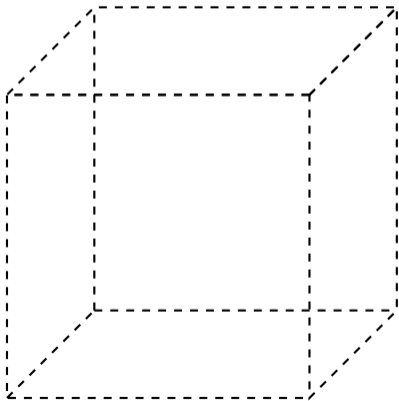


Nature Reviews | Cancer

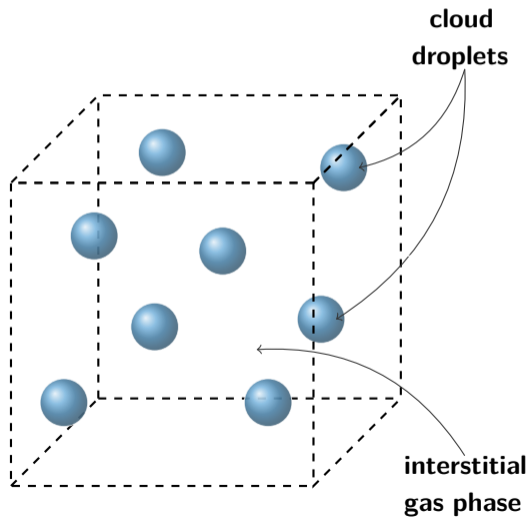
D. Tannant et al.: Targeting metabolic transformation for cancer therapy. Nat Rev Cancer 10: 267-277

Model Description

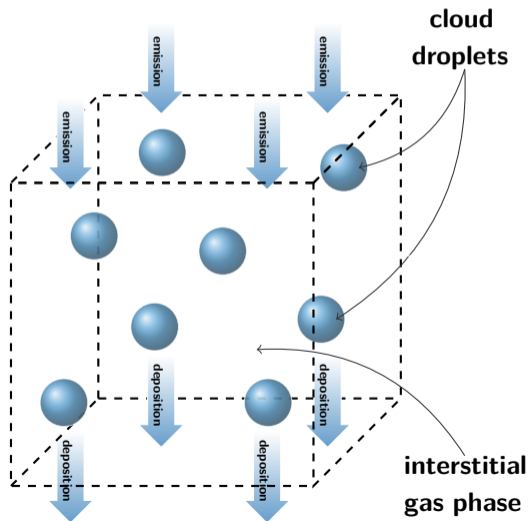
Box model framework



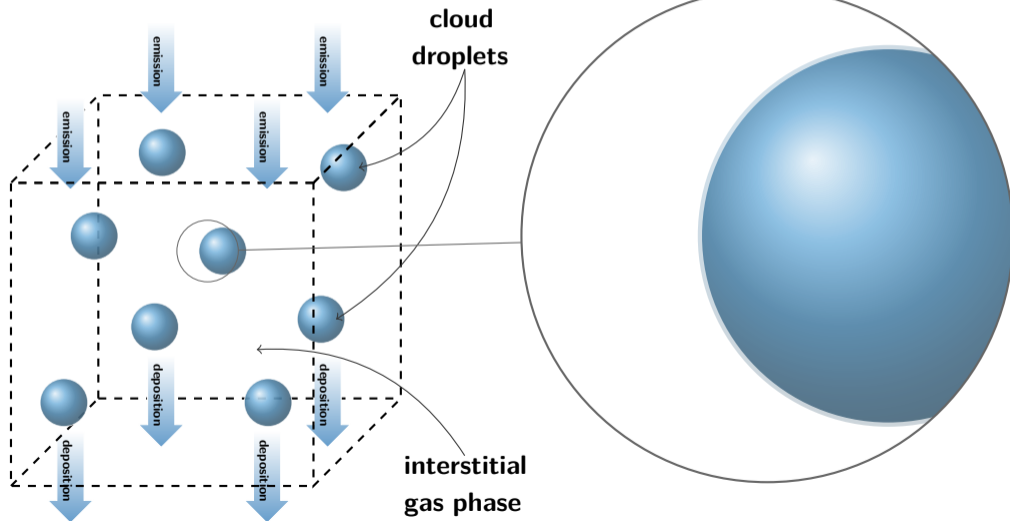
Box model framework



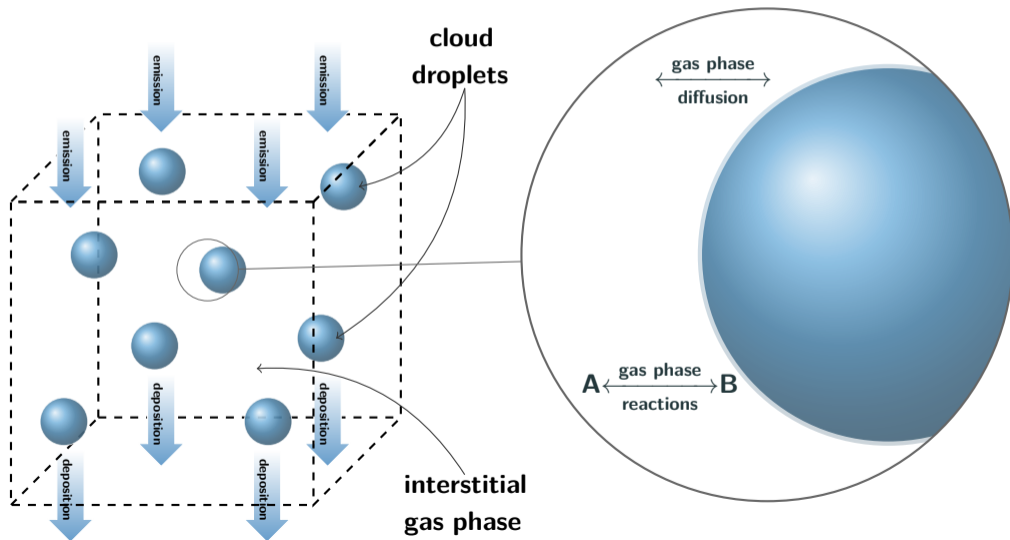
Box model framework



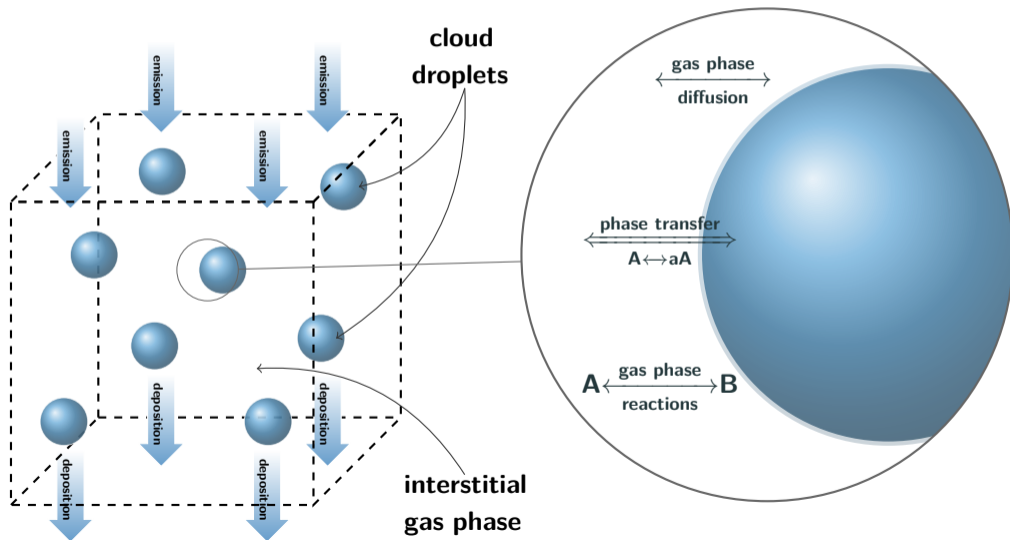
Box model framework



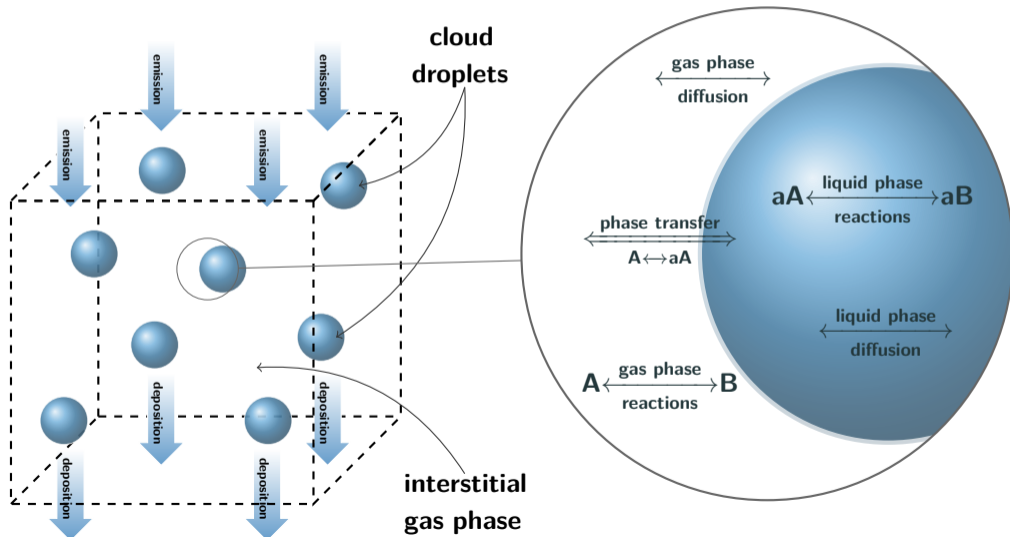
Box model framework



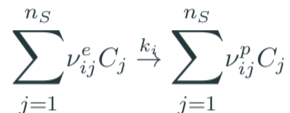
Box model framework



Box model framework



Mathematical formulation



(ν_{ij}^e) coefficients of the educts

(ν_{ij}^p) coefficients of the products

$\nu = \nu^p - \nu^e$ stoichiometric matrix (sparse)

k_i rate constant of reaction $i = 1, \dots, n_R$

C_j label of species $j = 1, \dots, n_S$

Model equations

rate of reaction i :
$$r_i(\mathbf{c}, T) = k_i(T) \cdot \prod_{j=1}^{n_S} c_j^{\nu_{ij}^e}, \quad i = 1, \dots, n_R$$

mass conservation:
$$\dot{c}_j = \sum_{i=1}^{n_R} \nu_{ij} r_i + c_j^{\text{emis}}, \quad j = 1, \dots, n_S$$

energy conservation:
$$\dot{T} = -\frac{1}{\bar{c}_v \cdot \rho} \sum_{j=1}^{n_S} \sum_{i=1}^{n_R} U_j [\nu_{ij} r_i + c_j^{\text{emis}}]$$

compact ODE form:
$$\dot{\mathbf{c}} = \boldsymbol{\nu}^T \mathbf{r} + \mathbf{c}^{\text{emis}}$$

$$\dot{T} = -\frac{1}{\bar{c}_v \rho} \mathbf{U}^T [\boldsymbol{\nu}^T \mathbf{r} + \mathbf{c}^{\text{emis}}]$$

- $U_j(T)$ molar internal energy of species j
 $C_{v,j}(T) = \partial U_j / \partial T$ constant volume specific heat of species j
 $\bar{c}_v(\mathbf{c}, T) = \sum_{j=1}^{n_S} (c_j C_{v,j})$ average mix specific heat at const. volume
 $\rho > 0$ average system density
 \mathbf{c}^{emis} emissions, deposition and dilution rates

Numerical Solver

Ordinary differential equation system

Dimension of the ODE system: $n = n_S + 1$, with $\dot{\mathbf{c}} \in \mathbb{R}^{n_S}$ and $\dot{T} \in \mathbb{R}$

$$y' = f(\mathbf{c}, T) = \begin{pmatrix} \dot{\mathbf{c}} \\ \dot{T} \end{pmatrix} = \begin{pmatrix} \nu^T r + c^{\text{emis}} \\ -\frac{1}{\bar{c}_v \cdot \rho} U^T [\nu^T r + c^{\text{emis}}] \end{pmatrix},$$

$$y(t = t_0) = (c_1^0, \dots, c_{n_S}^0, T^0)^T$$

Jacobian matrix of the ODE system:

$$J = \frac{\partial f(\mathbf{c}, T)}{\partial(\mathbf{c}, T)} = \left[\begin{array}{ccc|ccc} \ddots & & \ddots & \vdots & & \\ & \frac{\partial \dot{c}_l}{\partial c_j} & & \frac{\partial \dot{c}_l}{\partial T} & & \\ \ddots & & \ddots & \vdots & & \\ \hline \dots & \frac{\partial \dot{T}}{\partial c_j} & \dots & \frac{\partial \dot{T}}{\partial T} & & \end{array} \right], \quad l, j = 1, \dots, n_S.$$

Properties of kinetic differential equations

- The ODE system contains only **first order** derivatives dc/dt , which are usually **non-linear** functions of the concentrations.
- In general, several other concentrations influence the production rate of each species. \Rightarrow **coupled ODE system**
- The reaction rates differ several orders of magnitude. \Rightarrow **stiff ODE system**
- Simulation results of laboratory experiments do not depend on the wall clock time, but the results of atmospheric chemical models depend on the actual pressure, temperature and solar radiation \Rightarrow depend on the physical time.
- Some laboratory reactions can be (approximately) spatially homogeneous, but outside the laboratories most chemical reactions are spatially inhomogeneous. In most cases the transport of species and heat have to be taken into account.

Rosenbrock methods

An s -stage Rosenbrock method of order p is given by:

$$(I - \Delta t \gamma J) u_i = \Delta t f\left(y^{(n)} + \sum_{j=1}^{i-1} a_{ij} u_j\right) + \sum_{j=1}^{i-1} \gamma_{ij} u_j, \quad i = 1, \dots, s$$

$$y^{(n+1)} = y^{(n)} + \sum_{i=1}^s m_i u_i, \quad \hat{y}^{(n+1)} = y^{(n)} + \sum_{i=1}^s \hat{m}_i u_i$$

Butcher-Tableau:

$$\begin{array}{c|c|c}
 a & A & \Gamma \\
 \hline
 & m^T & \\
 & \hat{m}^T &
 \end{array}
 =
 \begin{array}{c|ccc|cc}
 a_1 & a_{11} & & & \gamma & \\
 \vdots & \vdots & \ddots & & \vdots & \ddots \\
 a_s & a_{s1} & \cdots & a_{ss} & \gamma_{s1} & \cdots & \gamma \\
 \hline
 & m_1 & \cdots & m_s & & & \\
 & \hat{m}_1 & \cdots & \hat{m}_s & & &
 \end{array}$$

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Butcher-Tableau:

$$\begin{array}{c|c|c} a & A & \Gamma \\ \hline & m^T & \\ & \hat{m}^T & \end{array} = \begin{array}{c|ccc|cc} a_1 & a_{11} & & & \gamma & \\ \vdots & \vdots & \ddots & & \vdots & \ddots \\ a_s & a_{s1} & \cdots & a_{ss} & \gamma_{s1} & \cdots & \gamma \\ \hline & m_1 & \cdots & m_s & & & \\ & \hat{m}_1 & \cdots & \hat{m}_s & & & \end{array}$$

← embedded formula

for error control: $\hat{p} = p - 1$

Analytical Jacobian formulation

Partial derivative of change in concentration with respect to concentration:

$$\left[\begin{array}{c|c} \frac{\partial \dot{\mathbf{c}}}{\partial \mathbf{c}} & \frac{\partial \dot{\mathbf{c}}}{\partial T} \\ \hline \frac{\partial \dot{T}}{\partial \mathbf{c}} & \frac{\partial \dot{T}}{\partial T} \end{array} \right]$$

$$J_{cc} = \frac{\partial f^c(\mathbf{c}, T)}{\partial \mathbf{c}} = \frac{\partial}{\partial \mathbf{c}} [\nu^T r + c^{\text{emis}}] = \nu^T \frac{\partial r(\mathbf{c}, T)}{\partial \mathbf{c}}$$

$$\Rightarrow \frac{\partial r_i}{\partial c_j} = \left(\frac{\nu_{ij}^e}{c_j} \right) \cdot k_i \cdot \prod_{l=1}^{n_S} c_l^{\nu_{il}^e} \Leftrightarrow \frac{\partial r_i}{\partial c_j} = \frac{r_i}{c_j} \cdot \nu_{ij}^e, \quad c_j \neq 0, \quad \forall j$$

$$\text{compact form: } J_{cc} = \nu^T D_r \nu^e D_c^{-1}$$

with:

$$D_r = \text{diag}(r_1, \dots, r_{n_R})$$

$$D_c^{-1} = \text{diag}(1/c_1, \dots, 1/c_{n_S})$$

Analytical Jacobian formulation

Partial derivative of change in concentration with respect to temperature:

$$\begin{bmatrix} \frac{\partial \dot{\mathbf{c}}}{\partial \mathbf{c}} & \frac{\partial \dot{\mathbf{c}}}{\partial T} \\ \frac{\partial \dot{T}}{\partial \mathbf{c}} & \frac{\partial \dot{T}}{\partial T} \end{bmatrix}$$

$$J_{cT} = \frac{\partial f^c(\mathbf{c}, T)}{\partial T} = \frac{\partial}{\partial T} [\nu^T r + c^{\text{emis}}] = \nu^T \frac{\partial r(\mathbf{c}, T)}{\partial T}$$

$$\Rightarrow \frac{\partial r_i}{\partial T} = \frac{\partial k_i(T)}{\partial T} \cdot \prod_{l=1}^{n_S} c_l^{\nu_{il}^e} \Leftrightarrow \frac{\partial r_i}{\partial T} = \underbrace{\frac{\partial k_i(T)}{\partial T} / k_i(T)}_{\mathbf{K}} \cdot r_i, \quad k_i \neq 0, \quad \forall i$$

compact form: $J_{cT} = \nu^T D_r \mathbf{K}$

with:

$$D_r = \text{diag}(r_1, \dots, r_{n_R})$$

$$\mathbf{K} = \left(\frac{\partial k_1}{\partial T} / k_1, \dots, \frac{\partial k_{n_R}}{\partial T} / k_{n_R} \right)^T$$

Analytical Jacobian formulation

Partial derivative of change in temperature with respect to concentration:

$$J_{Tc} = \frac{\partial f^T(\mathbf{c}, T)}{\partial \mathbf{c}} = \frac{\partial}{\partial \mathbf{c}} \left[-\frac{1}{\bar{c}_v \rho} U^T [\nu^T r + c^{\text{emis}}] \right]$$

$$\Rightarrow \frac{\partial \dot{T}}{\partial c_j} = -\frac{1}{\bar{c}_v} \left[\mathbf{C}_v \dot{T} + \sum_{l=1}^{N_S} U_j \frac{\partial \dot{c}_l}{\partial c_j} \right], \quad j = 1, \dots, n_S$$

$$\left[\begin{array}{c|c} \frac{\partial \dot{c}}{\partial \mathbf{c}} & \frac{\partial \dot{c}}{\partial T} \\ \hline \frac{\partial \dot{T}}{\partial \mathbf{c}} & \frac{\partial \dot{T}}{\partial T} \end{array} \right]$$

compact form: $J_{Tc} = -\frac{1}{\bar{c}_v \rho} \left[\mathbf{C}_v \dot{T} + U^T \nu^T D_r \nu^e D_c^{-1} \right]$

$$D_r = \text{diag}(r_1, \dots, r_{n_R})$$

with:

$$D_c^{-1} = \text{diag}(1/c_1, \dots, 1/c_{n_S})$$

$$\mathbf{C}_v = (\partial U_1 / \partial T, \dots, \partial U_{n_S} / \partial T)$$

Analytical Jacobian formulation

Partial derivative of change in temperature with respect to temperature:

$$J_{TT} = \frac{\partial f^T(\mathbf{c}, T)}{\partial T} = \frac{\partial}{\partial T} \left[-\frac{1}{\bar{c}_v \rho} U^T [\nu^T r + c^{\text{emis}}] \right]$$

$$\Rightarrow \frac{\partial \dot{T}}{\partial T} = -\frac{1}{\bar{c}_v} \left\{ \frac{1}{\bar{c}_v} \dot{T} \frac{\partial \bar{c}_v}{\partial T} + \sum_{l=1}^{N_S} \left[C_{v,l} \dot{c}_l + U_l \frac{\partial \dot{c}_l}{\partial T} \right] \right\}$$

$$\begin{bmatrix} \frac{\partial \dot{\mathbf{c}}}{\partial \mathbf{c}} & \frac{\partial \dot{\mathbf{c}}}{\partial T} \\ \frac{\partial \dot{T}}{\partial \mathbf{c}} & \frac{\partial \dot{T}}{\partial T} \end{bmatrix}$$

compact form: $J_{TT} = -\frac{1}{\bar{c}_v \rho} \left[\frac{1}{\bar{c}_v} \dot{T} \frac{\partial \bar{c}_v}{\partial T} + \mathbf{C}_v \dot{\mathbf{c}} + U^T \nu^T D_r \mathbf{K} \right]$

$$D_r = \text{diag}(r_1, \dots, r_{n_R})$$

with: $\mathbf{K} = \left(\frac{\partial k_1}{\partial T} / k_1, \dots, \frac{\partial k_{n_R}}{\partial T} / k_{n_R} \right)^T$

$$\mathbf{C}_v = (\partial U_1 / \partial T, \dots, \partial U_{n_S} / \partial T)$$

ODE system applied to Rosenbrock method

ODE applied to Rosenbrock method, **standard approach**

$$\left[\begin{array}{cc} I - \Delta t \gamma \overbrace{\nu^T D_r \nu^e D_c^{-1}}^{J_{cc}} & - \Delta t \gamma \overbrace{\nu^T D_r \mathbf{K}}^{J_{cT}} \\ - \Delta t \gamma \frac{1}{\bar{c}_v \rho} (\mathbf{C}_v \dot{T} + U^T J_{cc}) & 1 + \Delta t \gamma \frac{1}{\bar{c}_v \rho} \left(\frac{1}{\bar{c}_v} \frac{\partial \bar{c}_v}{\partial T} \dot{T} + \mathbf{C}_v \dot{c} + U^T J_{cT} \right) \end{array} \right] \begin{bmatrix} u_i \\ \tilde{u}_i \end{bmatrix} =$$

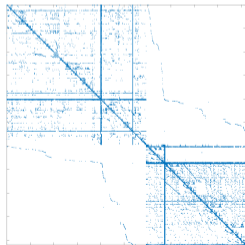
$$\Delta t \begin{bmatrix} \nu^T r_i + c^{\text{emis}} \\ -\frac{1}{\bar{c}_v \rho} U^T (\nu^T r_i + c^{\text{emis}}) \end{bmatrix} + \sum_{j=1}^{i-1} \gamma_{ij} \begin{bmatrix} u_j \\ \tilde{u}_j \end{bmatrix}$$

$$y^{\text{new}} = y^{\text{old}} + \sum_{i=1}^s m_i \begin{bmatrix} u_i \\ \tilde{u}_i \end{bmatrix}$$

ODE system applied to Rosenbrock method

ODE applied to Rosenbrock method, **standard approach**

$$\begin{bmatrix} I - \Delta t \gamma \overbrace{\nu^T D_r \nu^e D_c^{-1}}^{J_{cc}} & - \Delta t \gamma \overbrace{\nu^T D_r \mathbf{K}}^{J_{cT}} \\ - \Delta t \gamma \frac{1}{\bar{c}_v \rho} (\mathbf{C}_v \dot{T} + U^T J_{cc}) & 1 + \Delta t \gamma \frac{1}{\bar{c}_v \rho} \left(\frac{1}{\bar{c}_v} \frac{\partial \bar{c}_v}{\partial T} \dot{T} + \mathbf{C}_v \dot{c} + U^T J_{cT} \right) \end{bmatrix} \begin{bmatrix} u_i \\ \tilde{u}_i \end{bmatrix} =$$



$$\Delta t \begin{bmatrix} \nu^T r_i + c^{\text{emis}} \\ -\frac{1}{\bar{c}_v \rho} U^T (\nu^T r_i + c^{\text{emis}}) \end{bmatrix} + \sum_{j=1}^{i-1} \gamma_{ij} \begin{bmatrix} u_j \\ \tilde{u}_j \end{bmatrix}$$

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ODE system applied to Rosenbrock method

ODE applied to Rosenbrock method, **extended matrix approach**

$$\begin{bmatrix} D_r^{-1} & \gamma \nu^e & \gamma \mathbf{K} \\ \nu^T & \frac{1}{\Delta t} D_c & \mathbf{0} \\ \mathbf{0} & \gamma \mathbf{C}_v \dot{T} D_c + \frac{1}{\Delta t} U^T D_c & \frac{\bar{c}_v \rho}{\Delta t} + \frac{\gamma}{\bar{c}_v} \frac{\partial \bar{c}_v}{\partial T} \dot{T} + \gamma \mathbf{C}_v \dot{c} \end{bmatrix} \begin{bmatrix} x \\ u_i \\ \tilde{u}_i \end{bmatrix} =$$

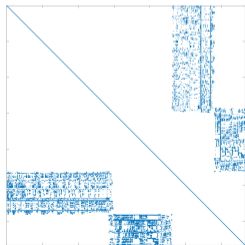
$$\begin{bmatrix} -D_r^{-1} r_i \\ c^{\text{emis}} \\ 0 \end{bmatrix} + \frac{1}{\Delta t} \sum_{j=1}^{i-1} \gamma_{ij} \begin{bmatrix} \mathbf{0} \\ u_j \\ (\bar{c}_v \rho \tilde{u}_j + U^T u_j) \end{bmatrix}$$

$$y^{\text{new}} = y^{\text{old}} + \sum_{i=1}^s m_i \begin{bmatrix} D_c u_i \\ \tilde{u}_i \end{bmatrix}$$

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$$y^{\text{new}} = y^{\text{old}} + \sum_{i=1}^s m_i \begin{bmatrix} D_c u_i \\ \tilde{u}_i \end{bmatrix}$$

Adaptive step size control

local error: $\hat{e}_j = y_j - \hat{y}_j$

scaling: $\text{scal}_j = \text{tol}_j^A + \max\{|y_j|, |\hat{y}_j|\} \cdot \text{tol}^R$

Maximum norm

$$\|\hat{e}\|_\infty = \max_j \left| \frac{\hat{e}_j}{\text{scal}_j} \right|$$

Euclidean norm

$$\|\hat{e}\|_2 = \sqrt{\sum_{j=1}^m \left(\frac{\hat{e}_j}{\text{scal}_j} \right)^2}$$

$$\Delta t^{\text{new}} = \begin{cases} \max \left\{ \Delta t_{\min}, \Delta t^{\text{old}} \cdot \max \{0.1, 0.8 \cdot \|\hat{e}\|^{-\delta}\} \right\}, & \text{if } \|\hat{e}\| > 1 \\ \min \left\{ \Delta t_{\max}, 0.8 \cdot \Delta t^{\text{old}} \cdot \|\hat{e}\|^{-\delta} \right\}, & \text{otherwise} \end{cases}$$

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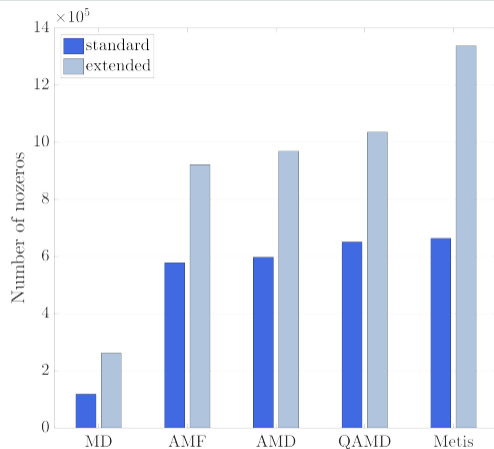
$\frac{1}{p+1}$

Sparse direct solver

- **given:** sparse matrix A , regular and unsymmetric
- **strategy to minimise computational effort:** symmetric permutation of A
 $\Rightarrow \bar{A} = PAP^T \rightarrow$ less fill-in
- **approaches finding P :**
 - minimum-degree (MD) by Markowitz
 - AMD, AMF, QAMD (varieties of MD)
 - Scotch, Metis (graph partitioning)

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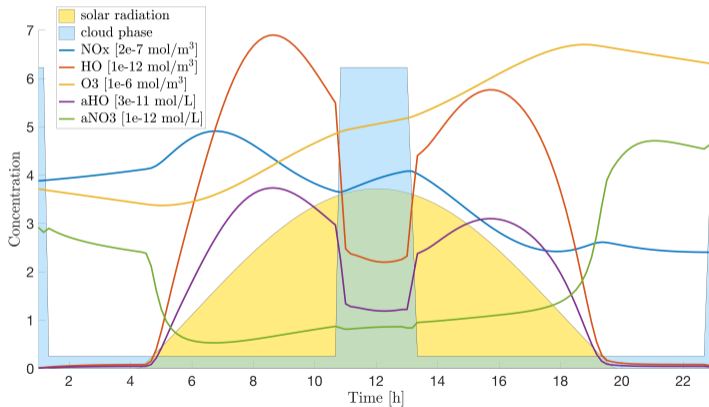


Comparison of ordering strategies applied to MCM3.2+CAPRAM4.0 mechanism

Profiles - tropospheric multiphase mechanism

RACM+CAPRAM2.4

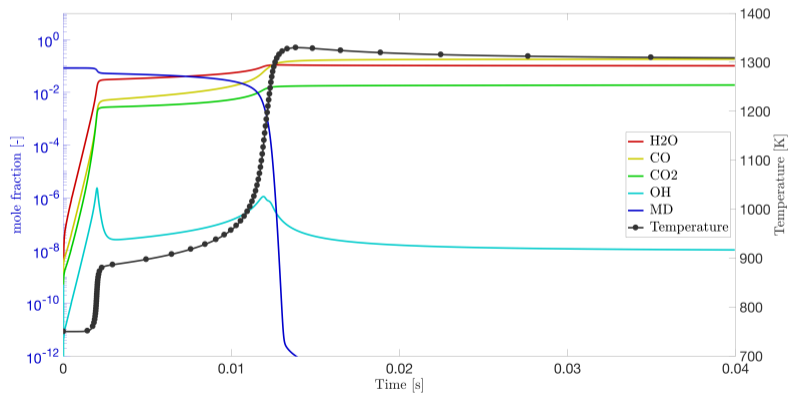
class	multiphase (gas, aqua)
scenario	urban
droplets	mono-disperse
n_S	250
n_R	787
tolerances	$\text{tol}_r = 10^{-3}$ $\text{tol}_a = 10^{-5}$ (gas) $\text{tol}_a = 10^{-5}$ (aqua)



Profiles - combustion mechanism

LLNL methyl-decanonate

class	gas phase combustion
T_0	750 [K]
p_0	2 [Bar]
n_S	2878
n_R	16831
tolerances	$\text{tol}_r = 10^{-4}$ $\text{tol}_a = 10^{-15}$ (gas) $\text{tol}_a = 10^{-1}$ (temp)



Summary and Further Work

Summary

Improving efficiency

- vectorised calculations using index sets \mathcal{I} , e.g. reaction rate constants:

$$k(\mathcal{I}_1) = A \cdot \exp(-E_A/(RT))$$

$$k(\mathcal{I}_2) = A' \cdot T^n \cdot \exp(E'_A/R \cdot (1/T - 1/T_{\text{ref}}))$$

- using sparse techniques (e.g sparse linear algebra, nnz \ll 1%)
- stable and robust integration schemes (large time steps, small errors)
- reducing the amount of queries to a minimum
- exploit compiler optimisations
 - preferred data structures: arrays, **NOT** objects, structs, linked lists
 - avoid procedure calls in loops with large iteration counts
- fast I/O routines, e.g. formatted meta-data files, unformatted data files

Further Work

Ideas

- parallel calculation of reaction rates and linear algebra (MPI, OpenMP, CAF)
- looking for improved ordering methods
- iterative methods for linear algebra
- simulate polydisperse systems
- implement micro physical scheme
- other features:
 - chemical mechanism parser: conversion between syntaxes (ChemKin format, .kpp, .sys)
 - automatic reduction of detailed chemical multiphase mechanisms