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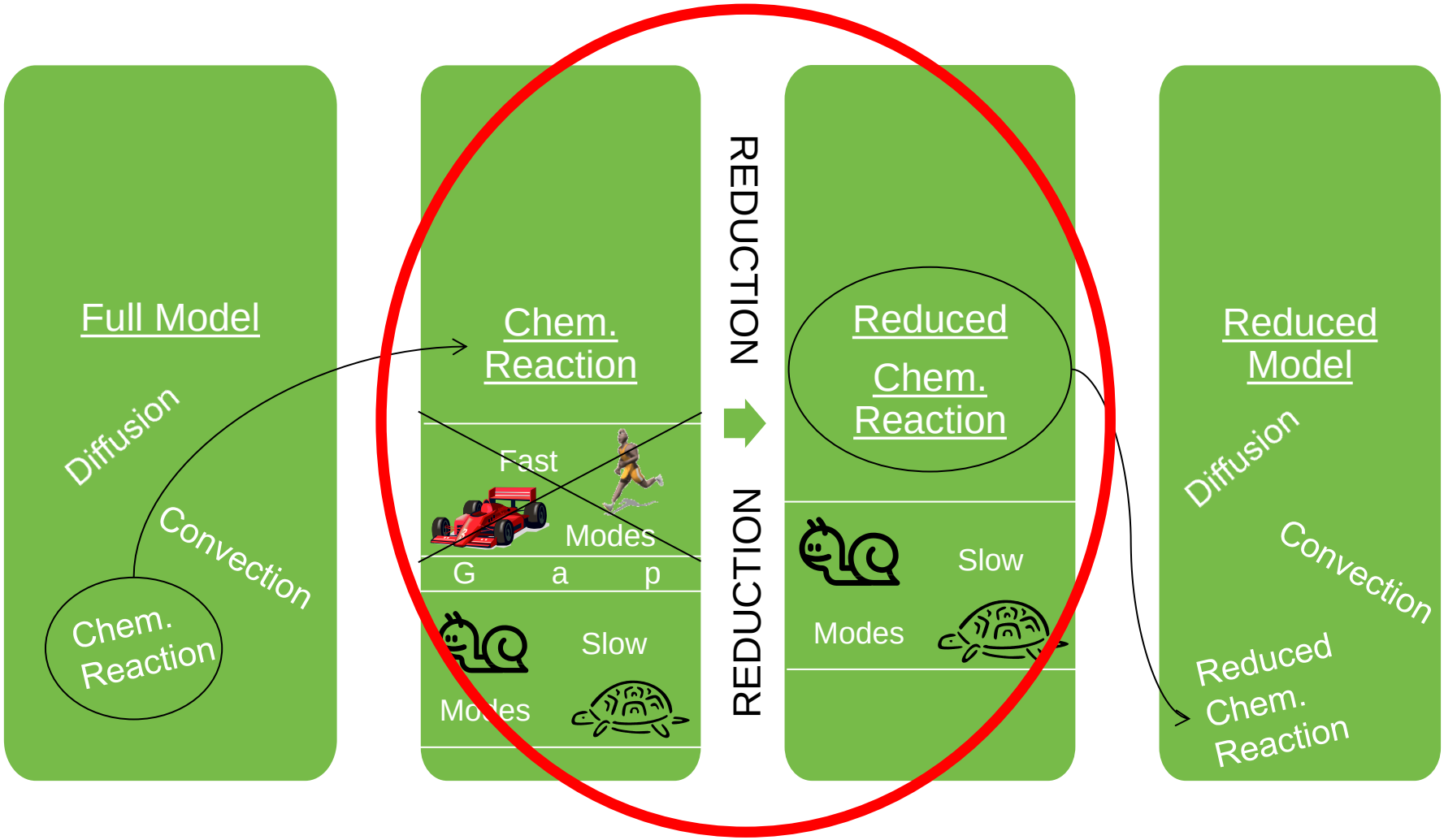
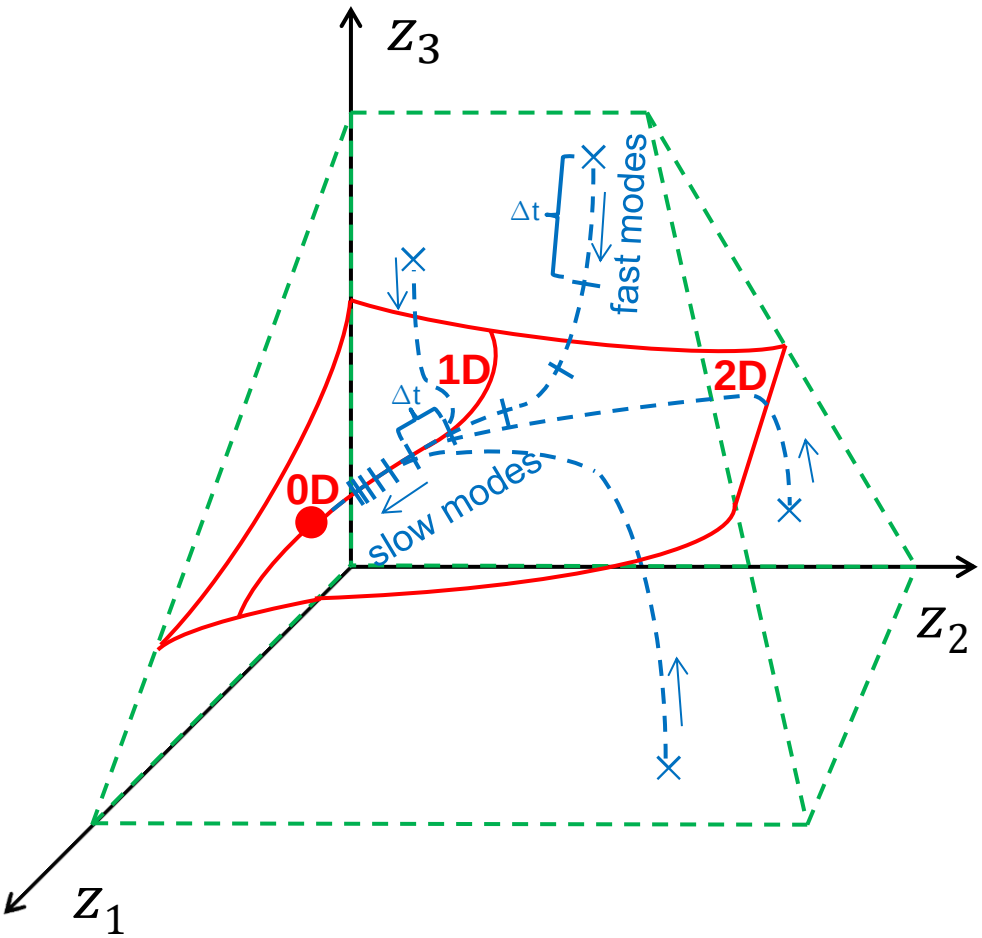
A Boundary Value View on the Reverse Trajectory-Based Optimization Approach for Kinetic Model Reduction

D. Lebiedz, J. Unger | June 19, 2013

Model Reduction

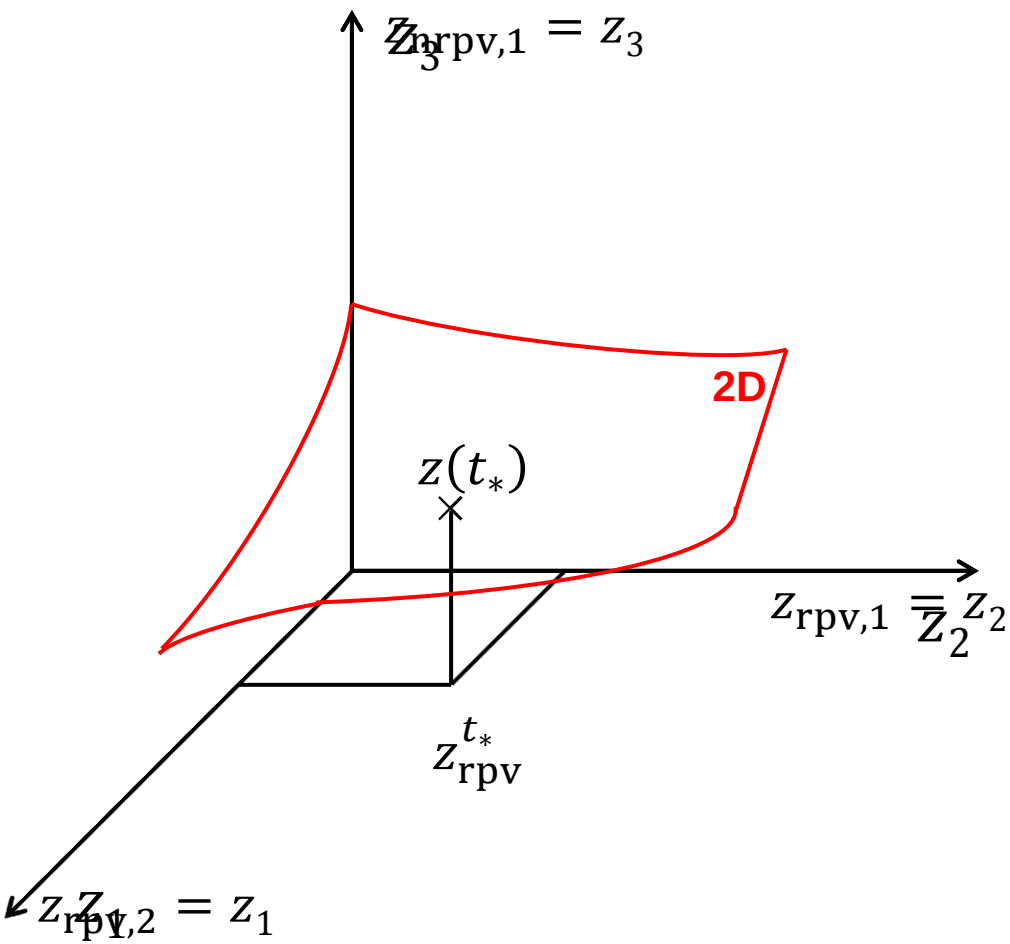


Phase Space Behavior



- 3D-Phase Space
- Constraints
- ODE-Solution
- Multiple Time Scales
- Appearance of SIMs

Species Reconstruction



- $z(t) = (z_i(t))_{i=1}^{n} \in \mathbb{R}^n$
- $z_{\mathrm{rpv}}(t) = (z_i(t))_{i \in I_{\mathrm{fixed}}} \in \mathbb{R}^{n_{\mathrm{rpv}}}$

  $z_{\mathrm{nrpv}}(t) = (z_i(t))_{i \notin I_{\mathrm{fixed}}} \in \mathbb{R}^{n_{\mathrm{nrpv}}}$
- $n_{\mathrm{rpv}} \triangleq$ Dimension of SIM
- Fixing $z_{\mathrm{rpv}}(t)$ at $t = t_*$
- Determination of

  $z_{\mathrm{nrpv}}(t_*) = h\big(z_{\mathrm{rpv}}(t_*)\big)$

Model Reduction: Linear Model

Reaction-Diffusion-Convection-PDE

$$\partial_t z(x,t) + \underbrace{v(x,t)\nabla z(x,t)}_{\text{Convection}} = \underbrace{\nabla \cdot \big(\mathrm{D}\nabla z(x,t)\big)}_{\text{Diffusion}} + \underbrace{S\big(z(x,t)\big)}_{\text{Reaction}}$$

?

$$z_1(t) = h(z_2(t)) = z_2(t)$$
$$\partial_t z_2(t) = -z_2(t) \rightarrow z_2(t) = \mathrm{c}_1 e^{-t}$$

SIM: $z_1(t) = h(z_2(t)) = z_2(t)$

$$z_1(t) = \mathrm{c}_1 e^{-t} + \cancel{\mathrm{c}_2 e^{(-1-\gamma)t}}$$
$$z_2(t) = \underbrace{\mathrm{c}_1 e^{-t}}_{\text{S.M.}} - \cancel{\underbrace{\mathrm{c}_2 e^{(-1-\gamma)t}}_{\text{F.M.}}}$$

$I_{\text{fixed}} = \{2\}$

Last Time (Corfu)…

Trajectory-Based Optimization Approach

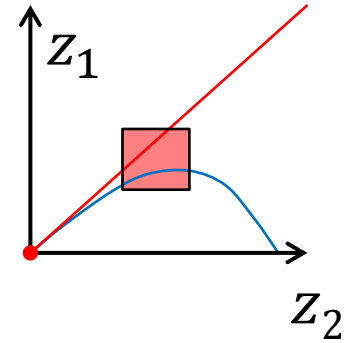
$$\min_{z(t)} \quad \int_{t_0}^{t_f} \left\| J_{S(z(t))} \cdot S(z(t)) \right\| \, dt$$

$$\text{s.t.} \quad z(t) = S(z(t))$$

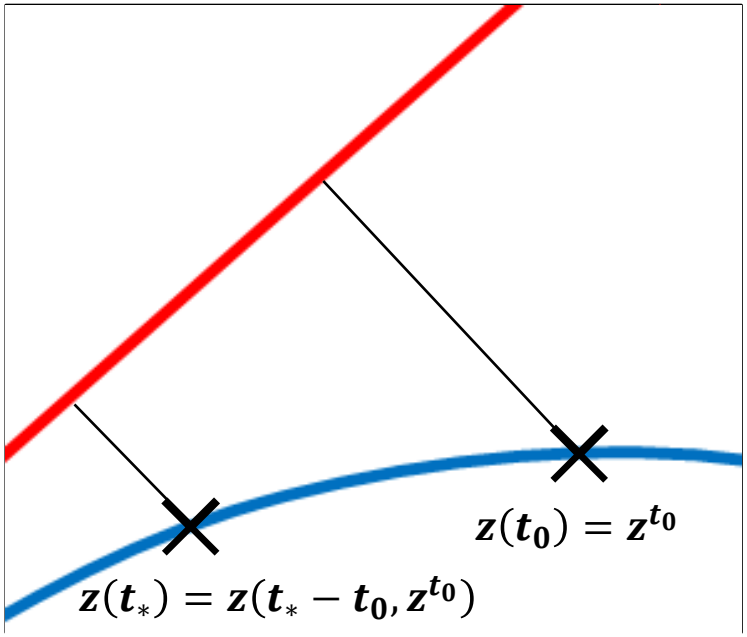
$$z_{rpv}(t_*) = z_{rpv}^{t_*}$$

WHY?

$$\lim_{t_0 \to -\infty} z(t_*) \in \mathbf{SIM}$$



Boundary Value Problem



BVP:

$$\partial_t z(t) = S\big(z(t)\big)$$
$$z_{\mathrm{rpv}}(t_*) = z_{\mathrm{rpv}}^{t_*}$$
$$z_{\mathrm{nrpv}}(t_0) = \mathrm{K} \in \mathbb{R}^{n_{\mathrm{nrpv}}}$$

$$\longrightarrow \quad \lim_{t_0 \to -\infty} z(t_*) \in \mathrm{SIM}$$

- $d(z(t_0), \mathrm{SIM}) > d(z(t_*), \mathrm{SIM}), \quad (t_0 < t_*)$
- $d(z(t_0), \mathrm{SIM}) \in \mathbb{R}, \quad t_* - t_0 = \infty$

$$\Rightarrow \quad d(z(t_*), \mathrm{SIM}) = 0$$

Choice of `K´

Zero-Derivative Principle[1]

$$\partial_t^m z_{\mathrm{nrpv}}(t) = 0 \quad |_{t=t_*}$$

$$\partial_t z(t) = S\big(z(t)\big)$$

$$z_{\mathrm{rpv}}(t_*) = z_{\mathrm{rpv}}^{t_*}$$

Trajectory-Based Optimization Approach[2]

$$\min_{\mathrm{z(t)}} \quad \int_{t_0}^{t_f} \left\| J_{S(z(t))} \cdot S\big(z(t)\big) \right\|_2^2 \mathrm{d}t$$

$$\text{s.t.} \qquad \partial_t z(t) = S\big(z(t)\big)$$

$$z_{\mathrm{rpv}}(t_*) = z_{\mathrm{rpv}}^{t_*}$$

Combination

$$\min_{\mathrm{z(t)}} \quad \|\partial_t^m z(t)\|_2^2 \quad |_{t=t_0}$$

$$\text{s.t.} \qquad \partial_t z(t) = S\big(z(t)\big)$$

$$z_{\mathrm{rpv}}(t_*) = z_{\mathrm{rpv}}^{t_*}$$

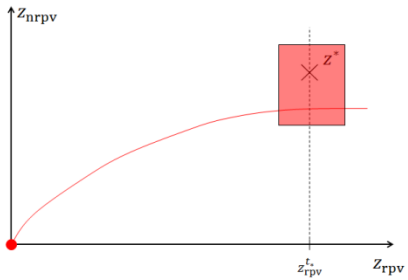
$$\lim_{t_0 \to -\infty} z(t_*) \in \mathrm{SIM}$$

$$\lim_{m \to \infty} z(t_*) \in \mathrm{SIM}$$

[1] A. Zagaris et al., *Analysis of the accuracy and convergence of equation-free projection to a slow manifold*, ESAIM: Math. Model. Num., 43 (2009)

[2] D. Lebiedz, J. Siehr, J.U., *A variational principle for computing slow invariant manifolds in dissipative dynamical systems*, SIAM J. Sci. Comput., 33 (2011)

Numerical Implementations: MORE



$$\min_{z(t)} \quad \left\|\partial_t^{m=2} z(t)\right\|_2^2 \;\Big|_{t=t_0=t_*}$$

$$\text{s.t.} \quad \cancel{\partial_t z(t) = S\big(z(t)\big)}$$

$$z_{\mathrm{rpv}}(t_*) = z_{\mathrm{rpv}}^{t_*}$$

$$h\big(z(t)\big) = 0$$

$$g\big(z(t)\big) \geq 0$$

Generalized **G**auss **N**ewon

+ **A**ctive **S**et **S**trategy

+ **Filter**

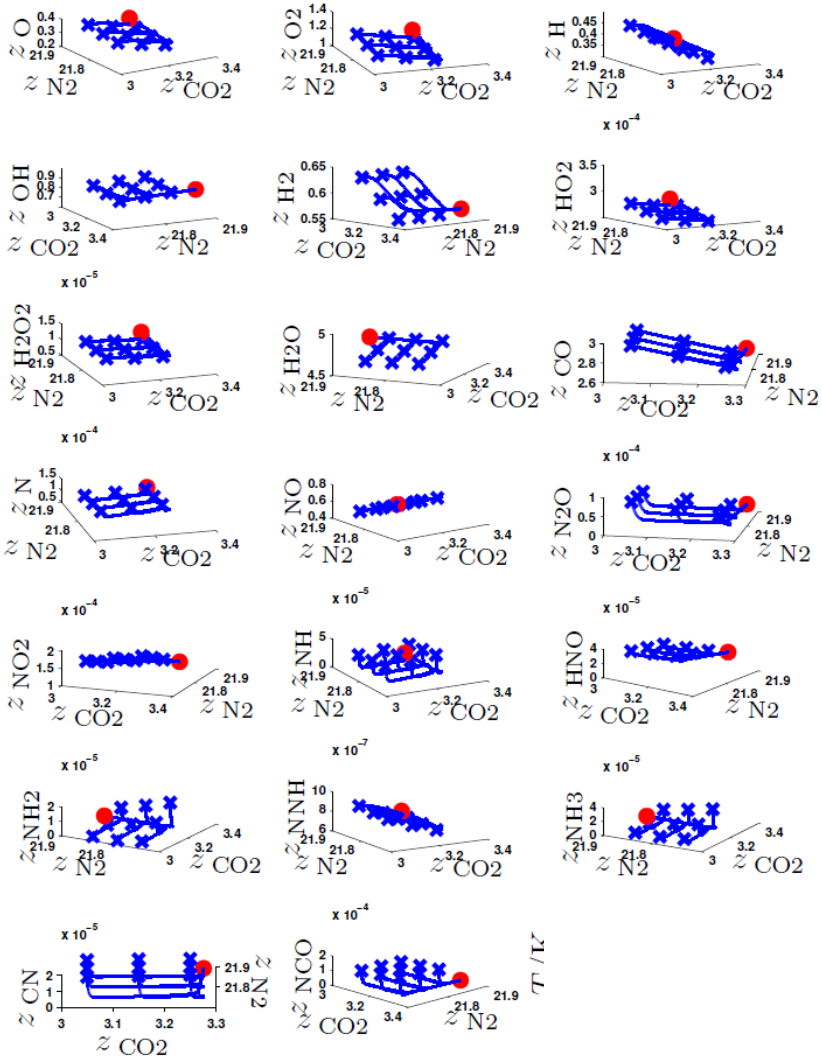
[1] A. V. Fiacco, *Sensitivity analysis for nonlinear programming using penalty methods*, Math. Program., 10 (1976)

Example[1,2,3]

$$n_{\text{spec}} = 22$$

$$n_{\text{reac}} = \sim 75$$

0.75 s

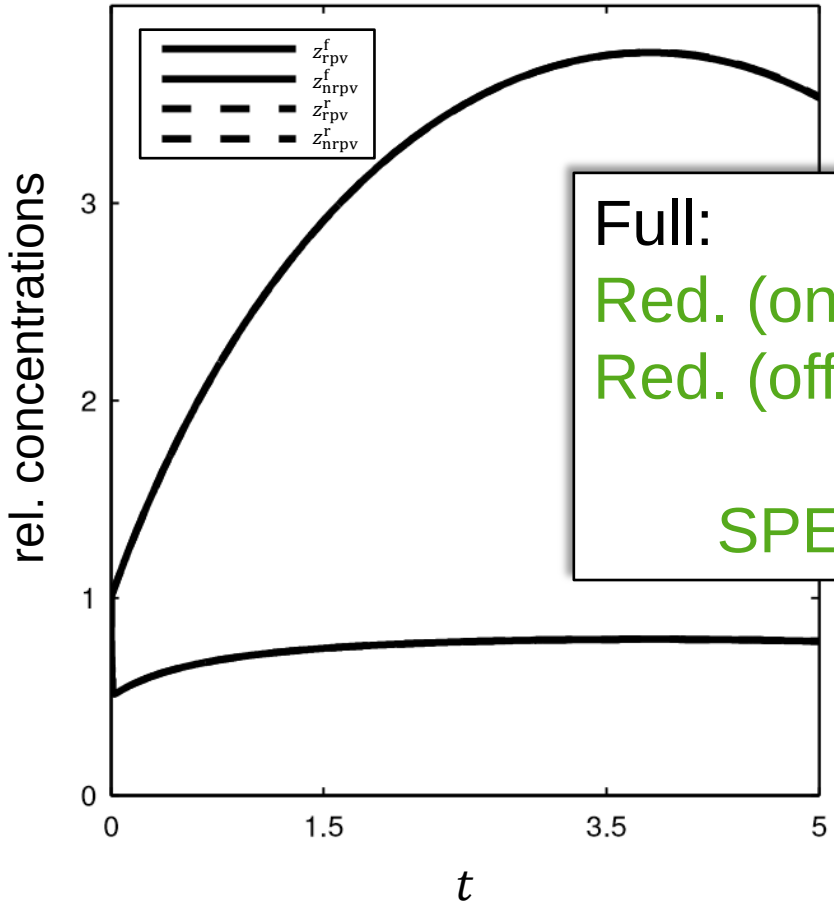


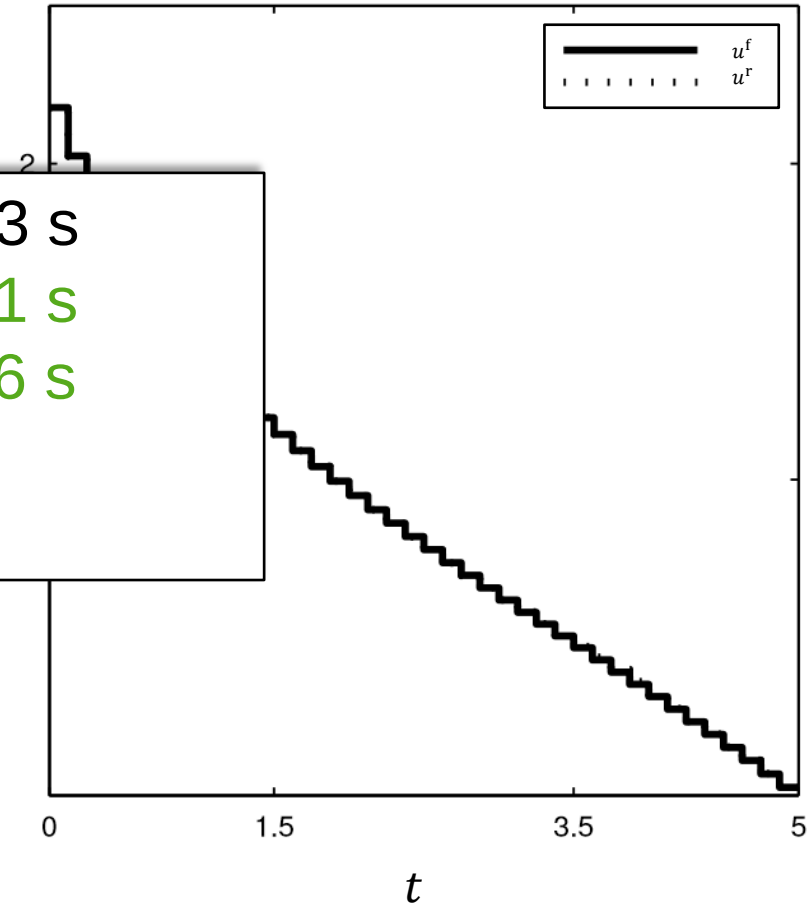
[1]J. Siehr, *Numerical optimization methods within a continuation strategy for the reduction of chemical combustion models*, Diss., Ruprecht-Karls-Universität Heidelberg, 2013

[2]D. Lebiedz, J. Siehr, *A continuation method for the efficient solution of parametric optimization problems in kinetic model reduction.* SIAM J. Sci. Comput. (in press)

[3]D. Lebiedz, J. Siehr, *An optimization approach to kinetic model reduction for combustion chemistry*, (submitted)

Optimal Control Problem[1]

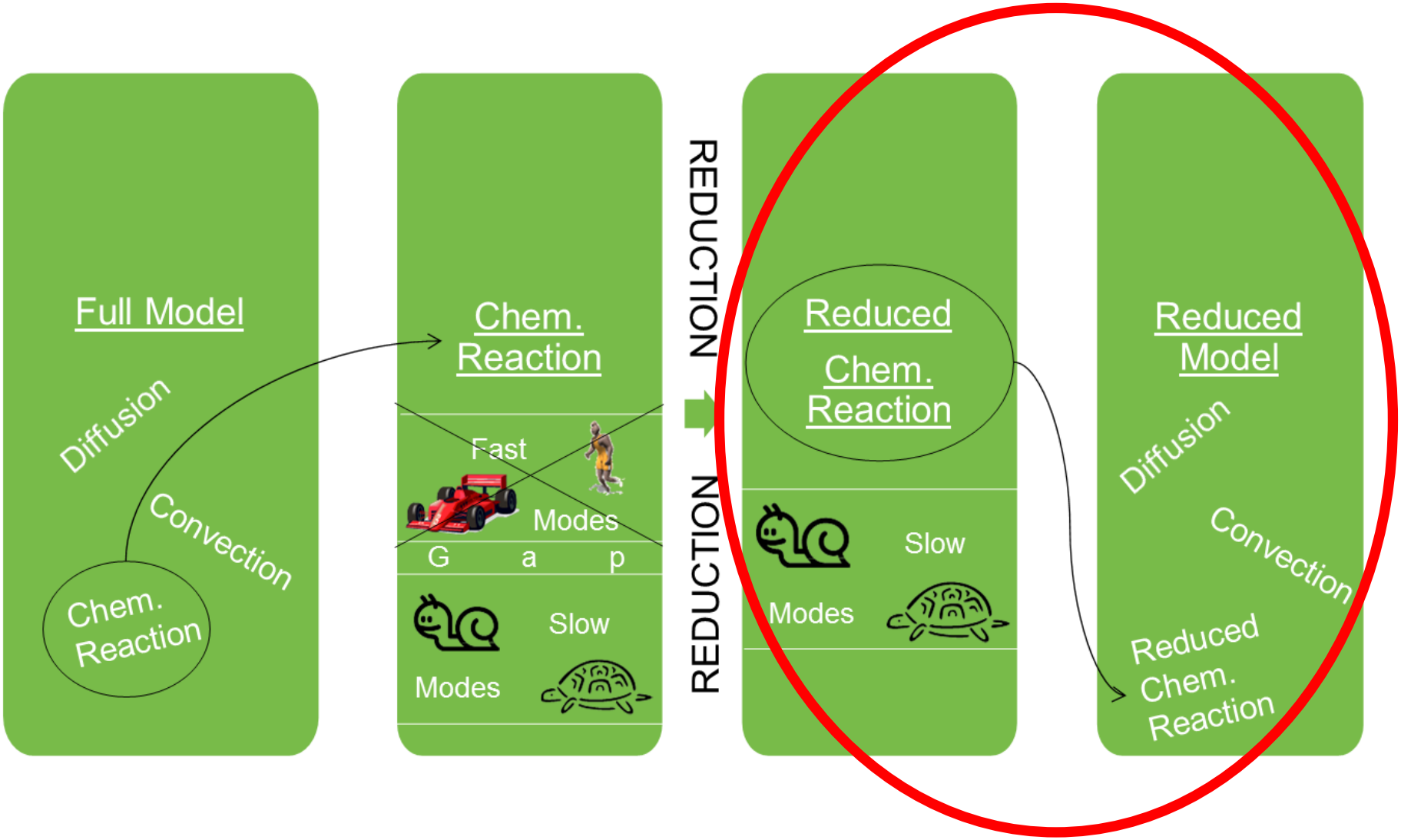




Full: 2.3 s
Red. (online): 2.1 s
Red. (offline): 0.6 s

SPEEDUP

[1] D.Lebiedz, M.Rehberg, *A numerical slow manifold approach to model reduction for optimal control of multiple time scale ODE*, (submitted), arXiv:1302.1759 [math.OC]


Full Model
Diffusion
Convection
Chem. Reaction
Chem. Reaction
Fast
Modes
G a p
Slow
Modes
REDUCTION
REDUCTION
Reduced Chem. Reaction
Slow
Modes
Reduced Model
Diffusion
Convection
Reduced Chem. Reaction

Problem Formulation

$$\partial_t z_1(x,t) + \cancel{\partial_x\big(v(x,t)z_1(x,t)\big)} + \mathrm{D}_1\partial_{xx}z_1(x,t) = S_1(z_1(x,t), z_2(x,t)) = -z_1$$
$$\partial_t z_2(x,t) + \cancel{\partial_x\big(v(x,t)z_2(x,t)\big)} + \mathrm{D}_2\partial_{xx}z_2(x,t) = S_2(z_1(x,t), z_2(x,t))$$

$$\partial_t z_1(x,t) + \partial_x\big(v(x,t)z_1(x,t)\big) + \mathrm{D}_1\partial_{xx}z_1(x,t) = S_1\big(z_1(x,t), \hat{h}(z_1(x,t))\big) = -\gamma z_2 + \frac{(\gamma - 1)z_1 + \gamma z_1^2}{(1+z_1)^2}$$

BV1: $z_1(x_0,t) = \mathrm{a}$; $z_1(x_1,t) = \mathrm{b}$ $\quad = 0 \quad = 1 \quad = 1 \quad = 1$

BV2: $z_2(x_0,t) = \mathrm{c}$; $z_2(x_1,t) = \mathrm{d}$ $\quad = 0.3 \quad = 0.7$

BV1: $z_1(x_0,t) = \mathrm{a}$; $z_1(x_1,t) = \mathrm{b}$ $\quad = 1$

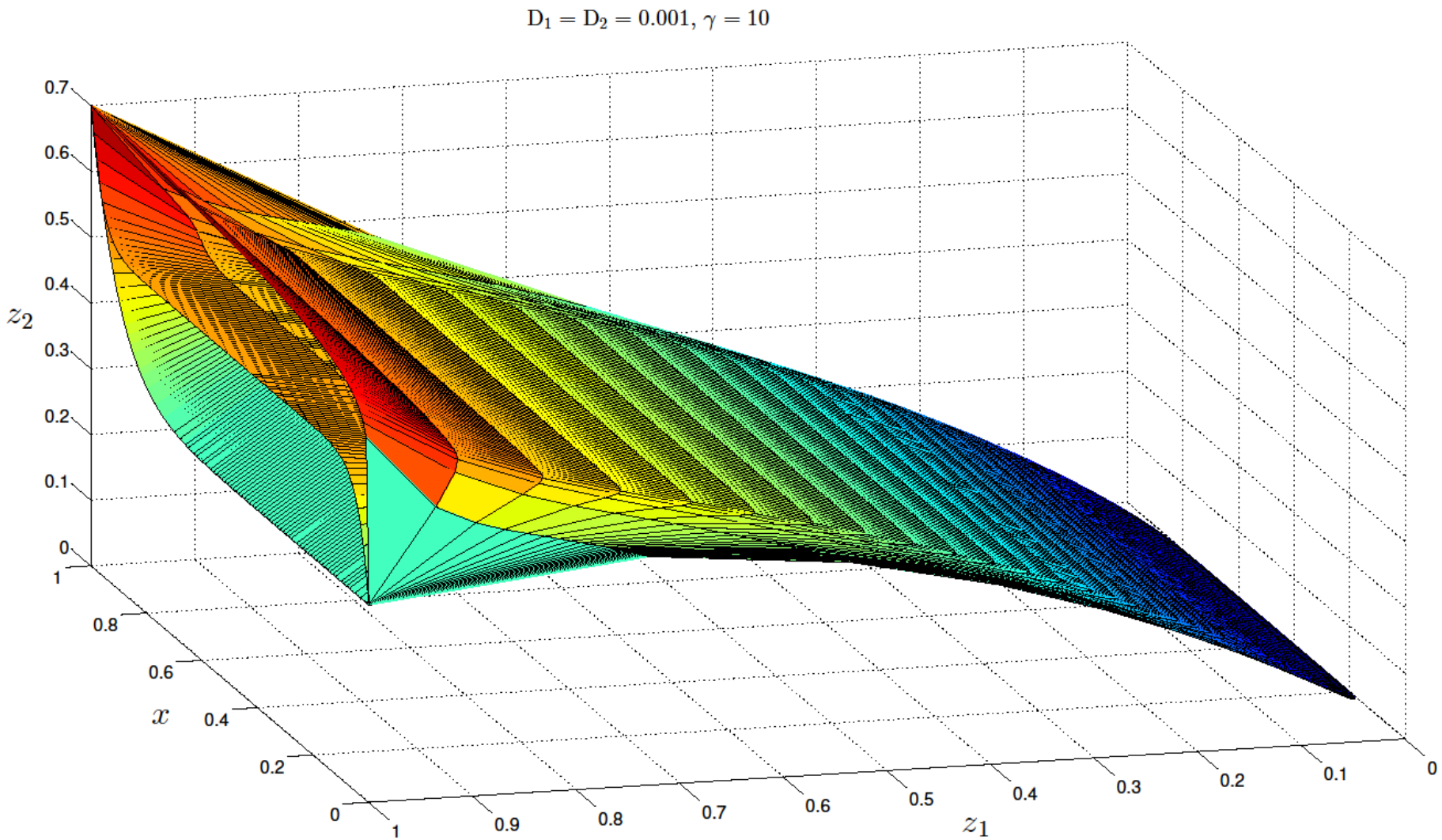
IV1: $z_1(x,t_*) = z_1^{t_*}(x)$; (s.t. BV1)

IV2: $z_2(x,t_*) = z_2^{t_*}(x)$; (s.t. BV2)

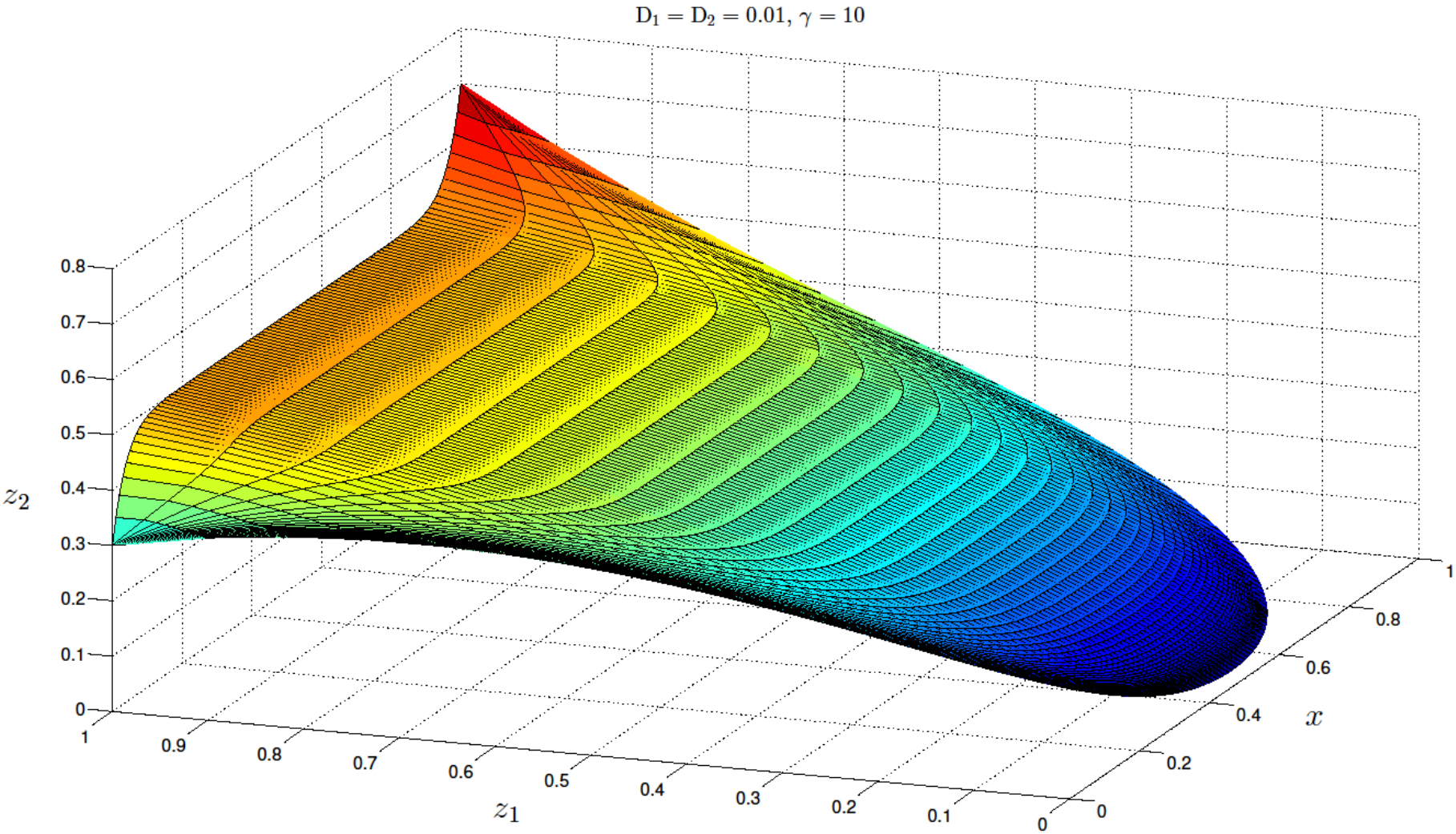
IV1: $z_1(x,t_*) = z_1^{t_*}(x)$; (s.t. BV1)

$z_2(x,t) = \hat{h}(z_1(x,t))$; (s.t. BV2)

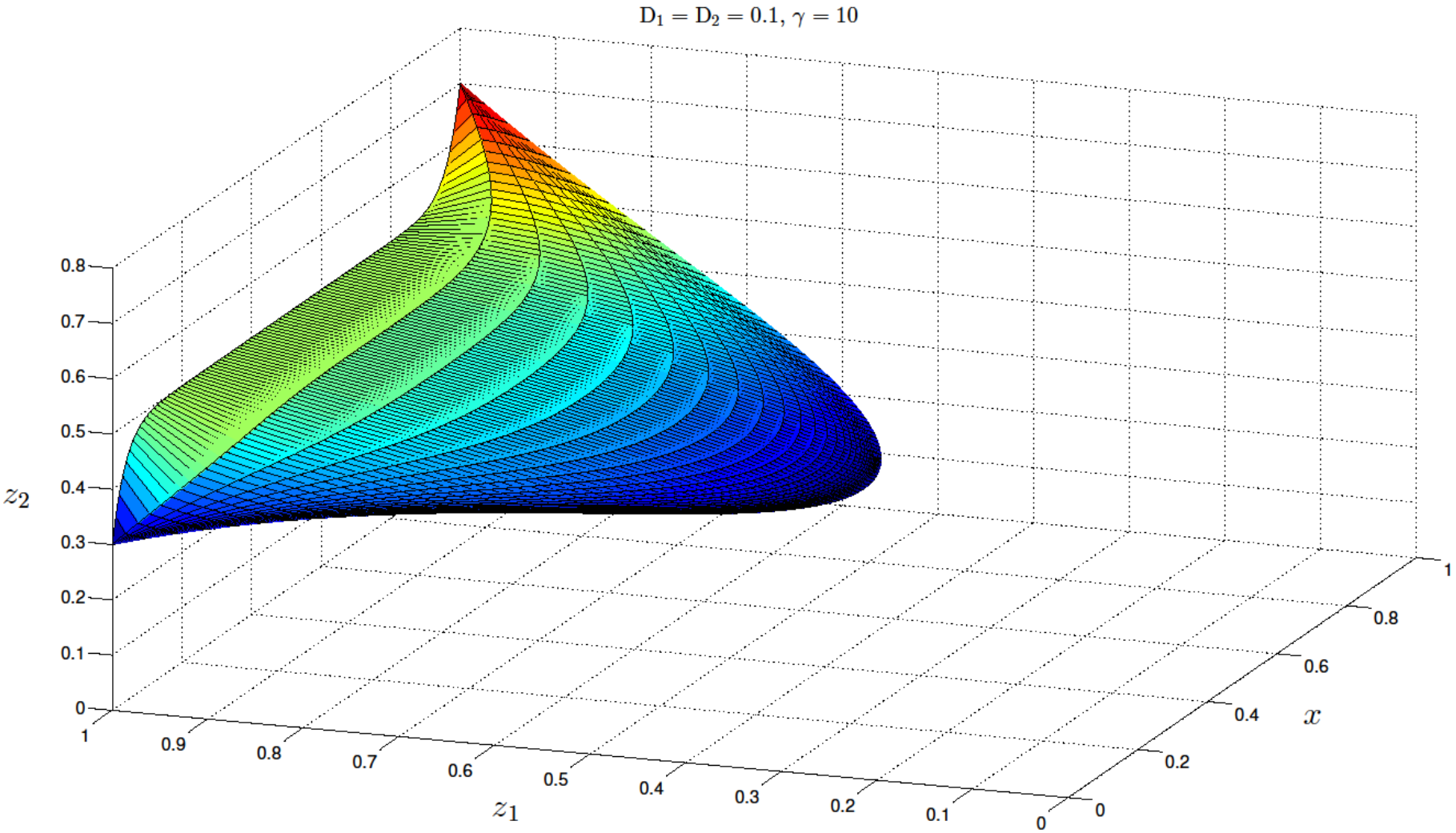
Example


$D_1 = D_2 = 0.001, \gamma = 10$
z_2
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
x
1
0.8
0.6
0.4
0.2
0
z_1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

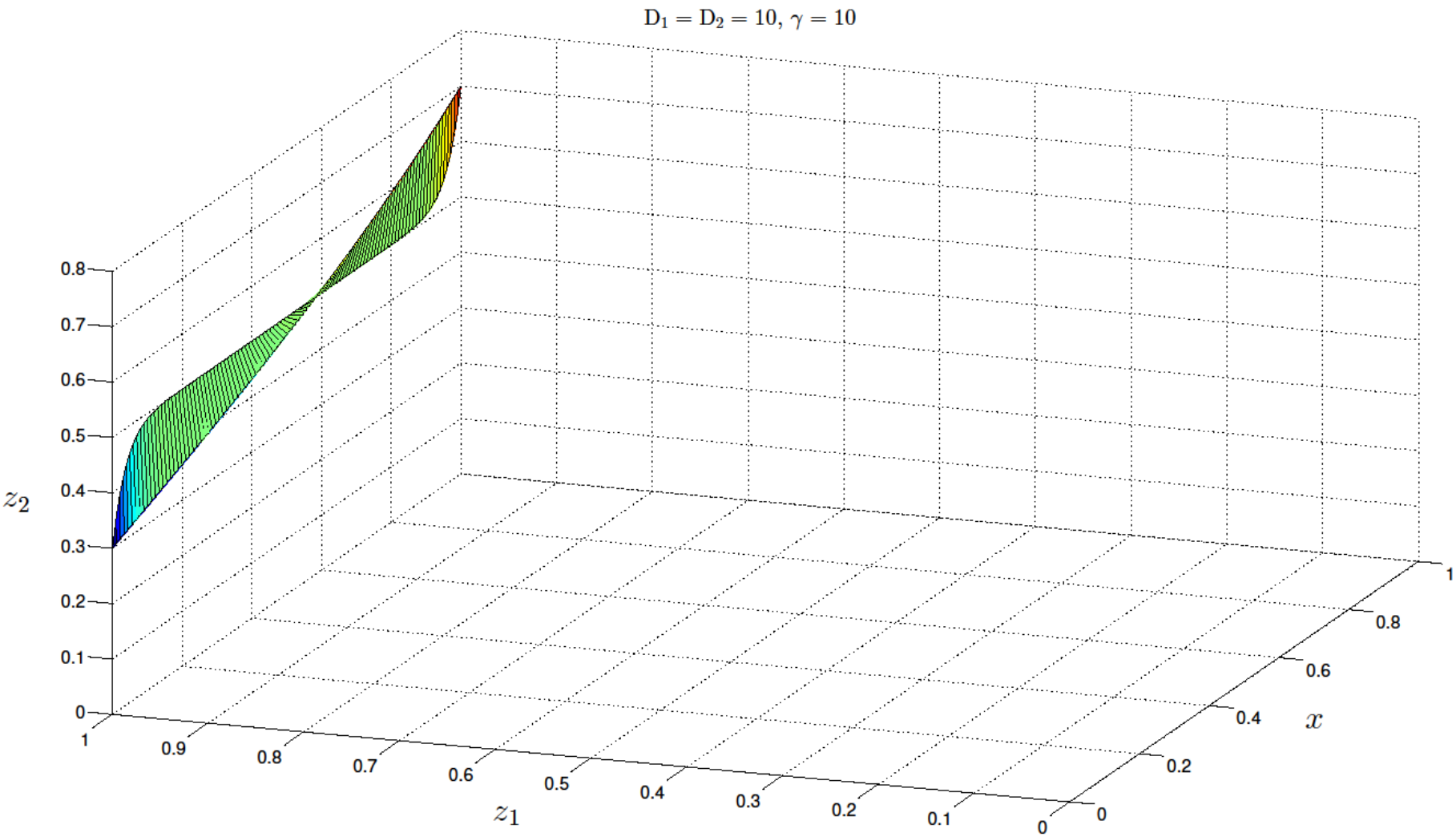
Example

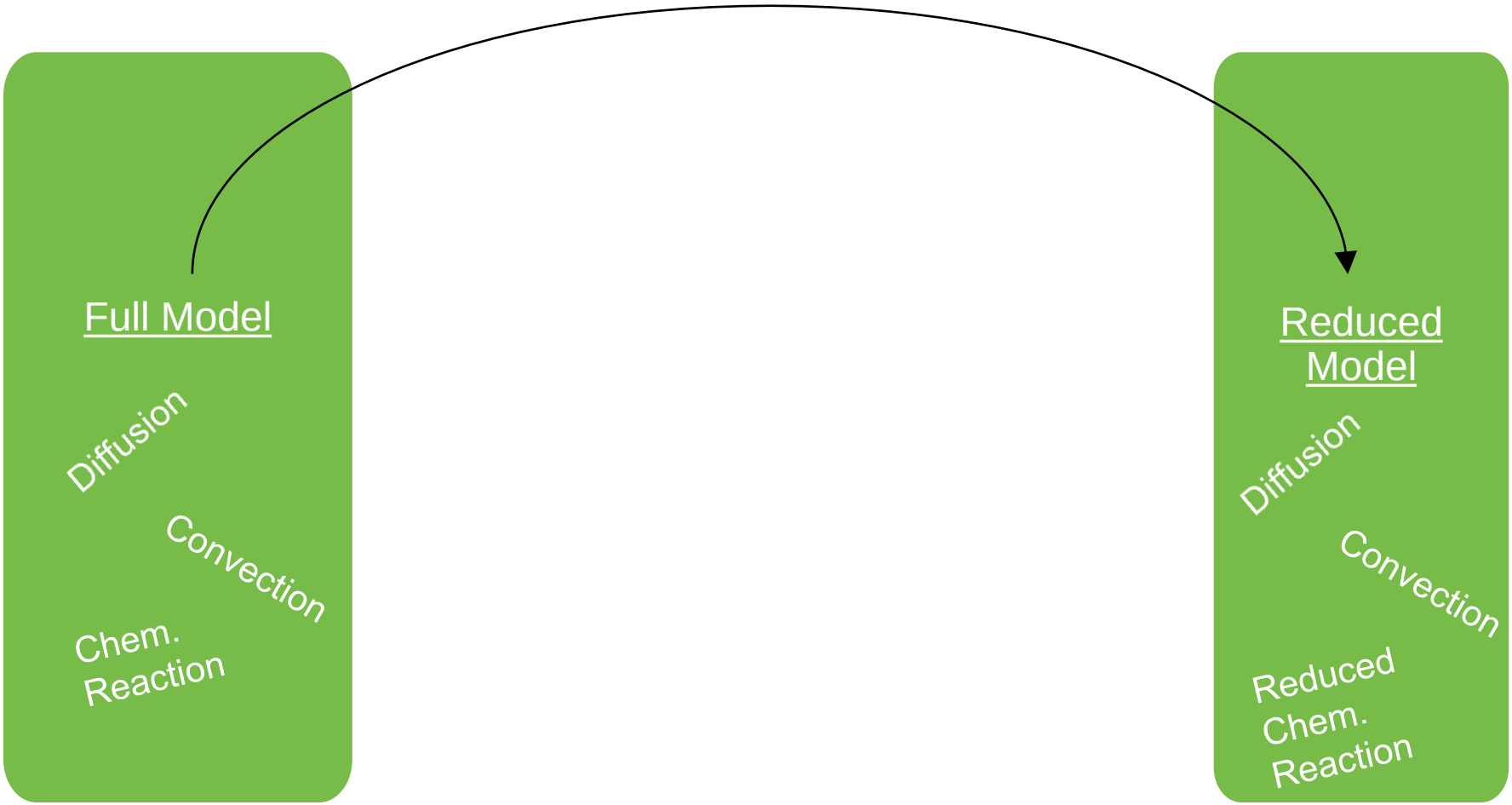

$D_1 = D_2 = 0.01, \gamma = 10$
z_2
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
z_1
0
0.2
0.4
0.6
0.8
1
x

Example


$D_1 = D_2 = 0.1, \gamma = 10$
z_2
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
z_1
0
0.2
0.4
0.6
0.8
1
x

Example


$D_1 = D_2 = 10,\ \gamma = 10$
z_2
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
z_1
0
0.2
0.4
0.6
0.8
1
x


Full Model
Diffusion
Convection
Chem. Reaction
Reduced Model
Diffusion
Convection
Reduced Chem. Reaction

BVP for PDE

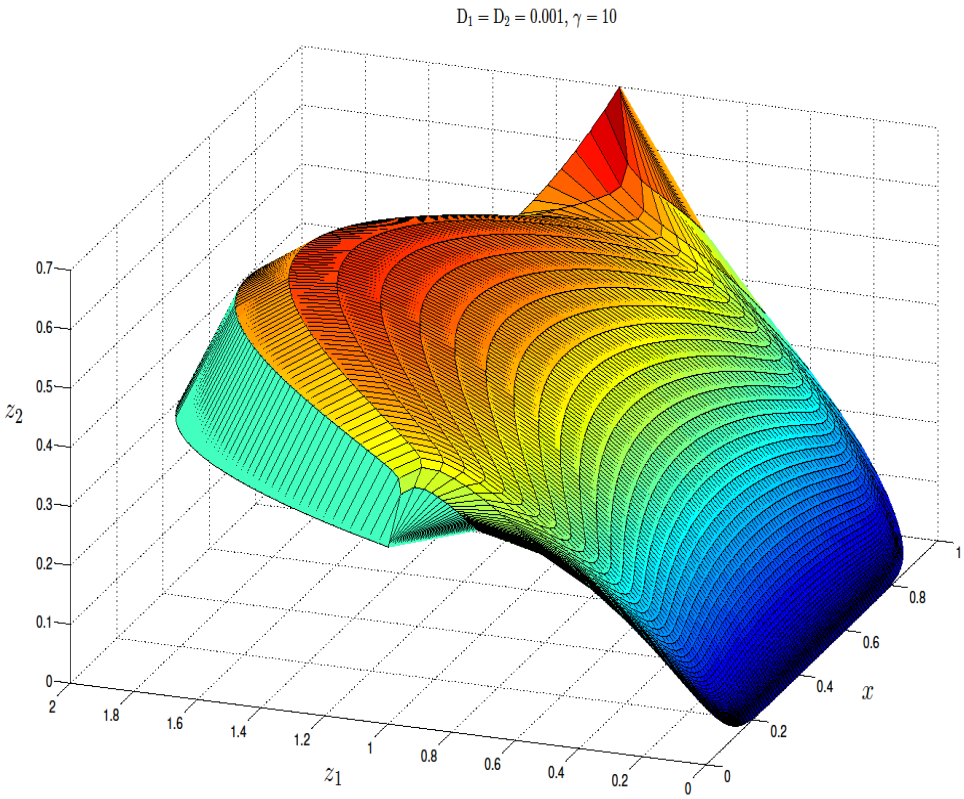
$$\partial_t z_1 + \mathrm{D}_1 \partial_{xx} z_1 = S_1(z_1, z_2)$$
$$\partial_t z_2 + \mathrm{D}_2 \partial_{xx} z_2 = S_2(z_1, z_2)$$

BV1: $z_1(x_0, t) = \mathrm{a}$; $z_1(x_1, t) = \mathrm{b}$

BV2: $z_2(x_0, t) = \mathrm{c}$; $z_2(x_1, t) = \mathrm{d}$

IV1: $z_1(x, t_*) = z_1^{t_*}(x)$; (s.t. BV1)

IV2: $z_2(x, t_0) = K(x)$; (s.t. BV2)



Summary

- BVP for Model Reduction
- Analytical Results
- ***MORE***: Numerically Efficient Model Reduction Toolbox
- Optimal Control of ODE
- First Insights into Reaction-Diffusion-Systems

Outlook

- Find ``Exact Criterion´´
- Numerical Tasks for Computing Realistic Large-Scale Combustion Mechanisms
- Find Function $\hat{h}$
- Computation of Reaction-Diffusion-SIMs
- Optimal Control of PDE

Thank you for your Attention!

Questions?