Tensor methods for higher-dimensional chemical Fokker-Planck equation

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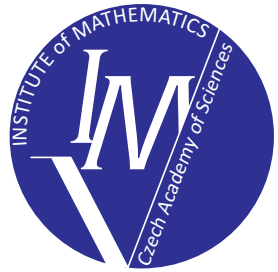


Joint work with Radek Erban and Shuohao Liao

Cambridge, 4–8 April 2016

Outline

1. Introduction
2. Well-posedness of Fokker-Planck equation
3. Tensor methods
4. Error estimation

General chemical system

Well mixed reactor, N chemical species, M reactions:

$$\sum_{i=1}^{N} \nu_{ji}^{\mathrm{r}} X_i \xrightarrow{k_j} \sum_{i=1}^{N} \nu_{ji}^{\mathrm{p}} X_i, \qquad j = 1, 2, \ldots, M$$

Markov proces:

Reaction j occurs in time interval $(t, t + \mathrm{d}t)$ with probability $\alpha_j(\mathbf{X}(t))\,\mathrm{d}t$, where

- $\mathbf{X}(t) = [X_1(t), \ldots, X_N(t)]$
- $X_i(t)$ are numbers of molecules at time t, $i = 1, \ldots, N$
- $\alpha_j(\mathbf{x}) = k_j \prod_{i=1}^{N} \binom{x_i}{\nu_{ji}^{\mathrm{r}}}$ are propensities, $j = 1, \ldots, M$
- $\nu_{ji} = \nu_{ji}^{\mathrm{p}} - \nu_{ji}^{\mathrm{r}}$, change of X_i during reaction j

Probability distribution

Quantity of interest:

$p(\mathbf{x}, t) = \Pr(\mathbf{X}(t) = \mathbf{x})$

Exact description

- Stochastic simulations (Gillespie algorithm)
- Chemical master equation

Approximate description

- Stochastic simulations (Langevin equation)
- Chemical Fokker–Planck equation

Chemical Fokker–Planck equation

$$\frac{\partial p}{\partial t}(\mathbf{x},t) = \sum_{i=1}^{N}\sum_{k=1}^{N}\frac{\partial^2}{\partial x_i \partial x_k}\left[\left(\frac{1}{2}\sum_{j=1}^{M}\nu_{ji}\nu_{jk}\alpha_j(\mathbf{x})\right)p(\mathbf{x},t)\right] - \sum_{i=1}^{N}\frac{\partial}{\partial x_i}\left[\left(\sum_{j=1}^{M}\nu_{ji}\alpha_j(\mathbf{x})\right)p(\mathbf{x},t)\right]$$

Vector notation

$$\frac{\partial p}{\partial t}(\mathbf{x},t) = \operatorname{div}\left[\operatorname{div}(\mathcal{A}(\mathbf{x})p(\mathbf{x},t)) - \mathbf{b}(\mathbf{x})p(\mathbf{x},t)\right]$$

- $\mathcal{A} \in \mathbb{R}^{N\times N}$, $\mathcal{A}_{ik}(\mathbf{x}) = \frac{1}{2}\sum_{j=1}^{M}\nu_{ji}\nu_{jk}\alpha_j(\mathbf{x})$
- $\mathbf{b} \in \mathbb{R}^{N}$, $b_i(\mathbf{x}) = \sum_{j=1}^{M}\nu_{ji}\alpha_j(\mathbf{x})$

2. Well-posedness of chemical Fokker-Planck equation

Ellipticity

$$\frac{\partial p}{\partial t} = \operatorname{div}\left[\operatorname{div}(\mathcal{A}p) - \mathbf{b}p\right]$$

Fokker-Planck operator is elliptic if $\mathcal{A}(\mathbf{x})$ is symmetric positive definite.

Notice: $\mathcal{A}_{ik}(\mathbf{x}) = \frac{1}{2}\sum_{j=1}^{M} \nu_{ji}\alpha_j(\mathbf{x})\nu_{jk} \quad \Longrightarrow \quad \mathcal{A} = \frac{1}{2}\boldsymbol{\nu}^T\boldsymbol{\alpha}\boldsymbol{\nu}$

- $\boldsymbol{\nu} \in \mathbb{R}^{M\times N}$, ν_{ji} are stoichiometric coefficients
- $\boldsymbol{\alpha} \in \mathbb{R}^{M\times M}$, $\boldsymbol{\alpha} = \operatorname{diag}(\alpha_1, \ldots, \alpha_M)$

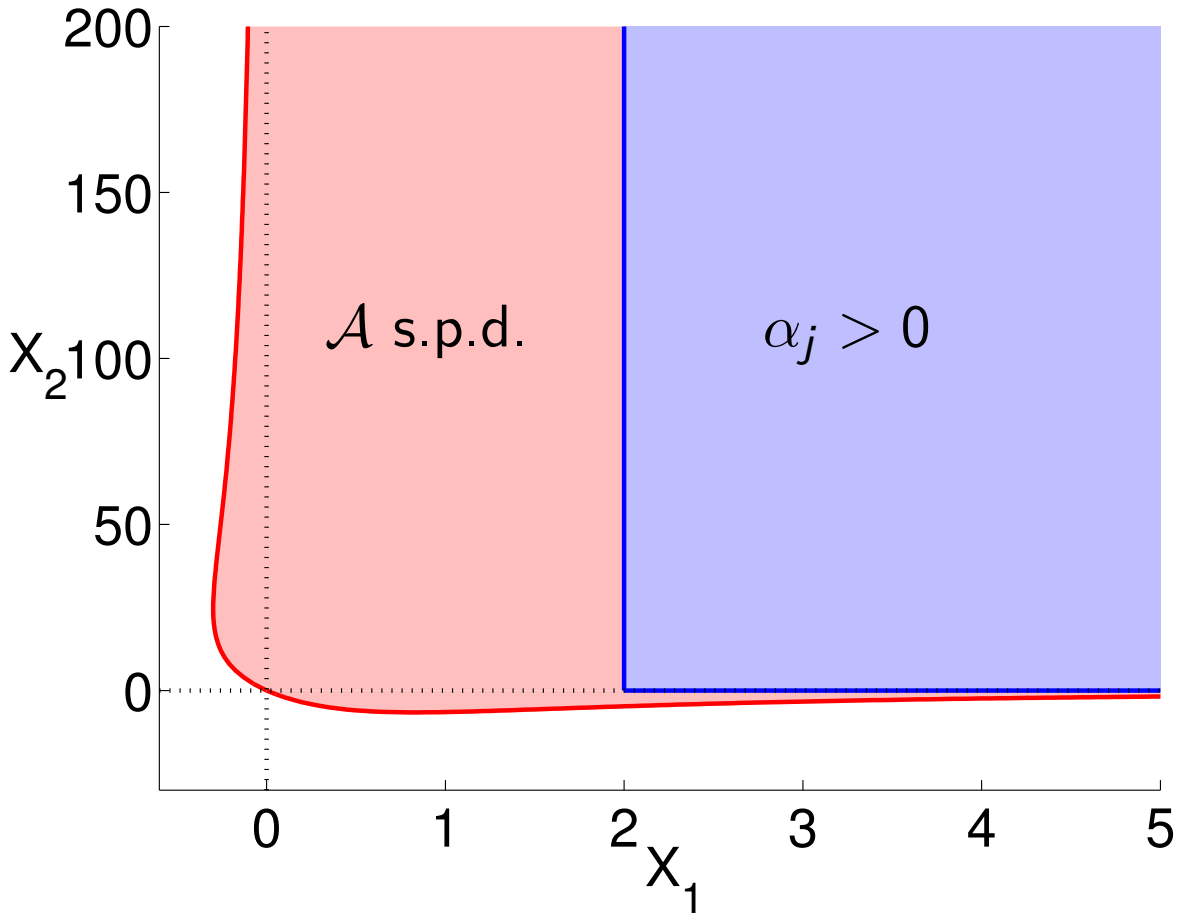
Lemma.
Let N columns of $\boldsymbol{\nu} \in \mathbb{R}^{M\times N}$ be linearly independent.
Let $\alpha_j > 0$ for all $j = 1, 2, \ldots, M$.
Then $\mathcal{A} = \frac{1}{2}\boldsymbol{\nu}^T\boldsymbol{\alpha}\boldsymbol{\nu}$ is symmetric positive definite.

Proof. Let $\mathbf{y} \in \mathbb{R}^N$, $\mathbf{y} \neq 0$. Then $\mathbf{z} = \boldsymbol{\nu}\mathbf{y} \neq 0$. Thus,

$$\mathbf{y}^T\mathcal{A}\mathbf{y} = \frac{1}{2}\mathbf{y}^T\boldsymbol{\nu}^T\boldsymbol{\alpha}\boldsymbol{\nu}\mathbf{y} = \frac{1}{2}\mathbf{z}^T\boldsymbol{\alpha}\mathbf{z} > 0.$$

Example: SNIPER

$$\emptyset \xrightarrow{k_1} X_2$$
$$X_2 \xrightarrow{k_2} X_1$$
$$X_1 \xrightarrow{k_3} \emptyset$$
$$2X_1 \xrightarrow{k_4} 3X_1$$
$$3X_1 \xrightarrow{k_5} 2X_1$$
$$X_1 + X_2 \xrightarrow{k_6} X_1 + 2X_2$$
$$2X_1 + X_2 \xrightarrow{k_7} 2X_1$$



[R. Erban, S.J. Chapman, I.G. Kevrekidis, T. Vejchodsky, SIAM J. Appl. Math. 2009.]

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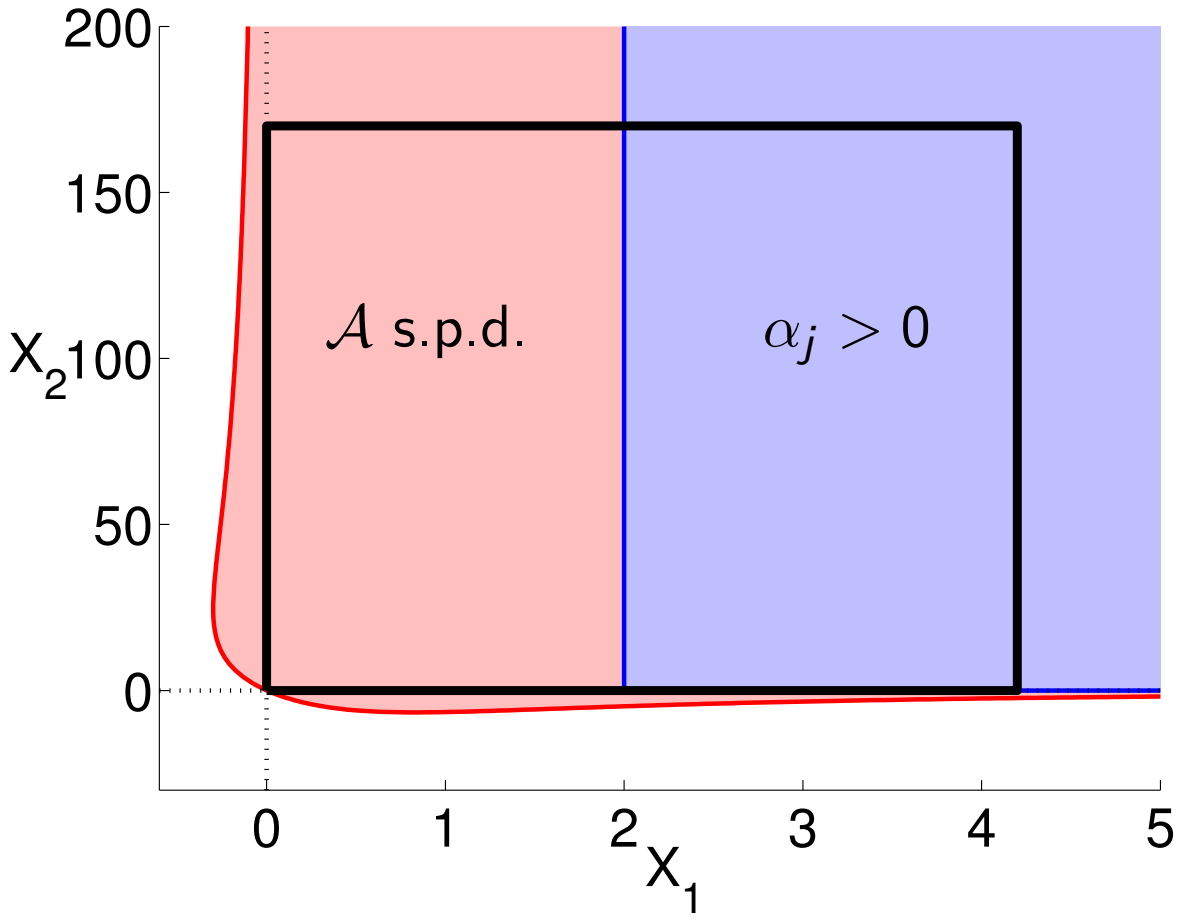

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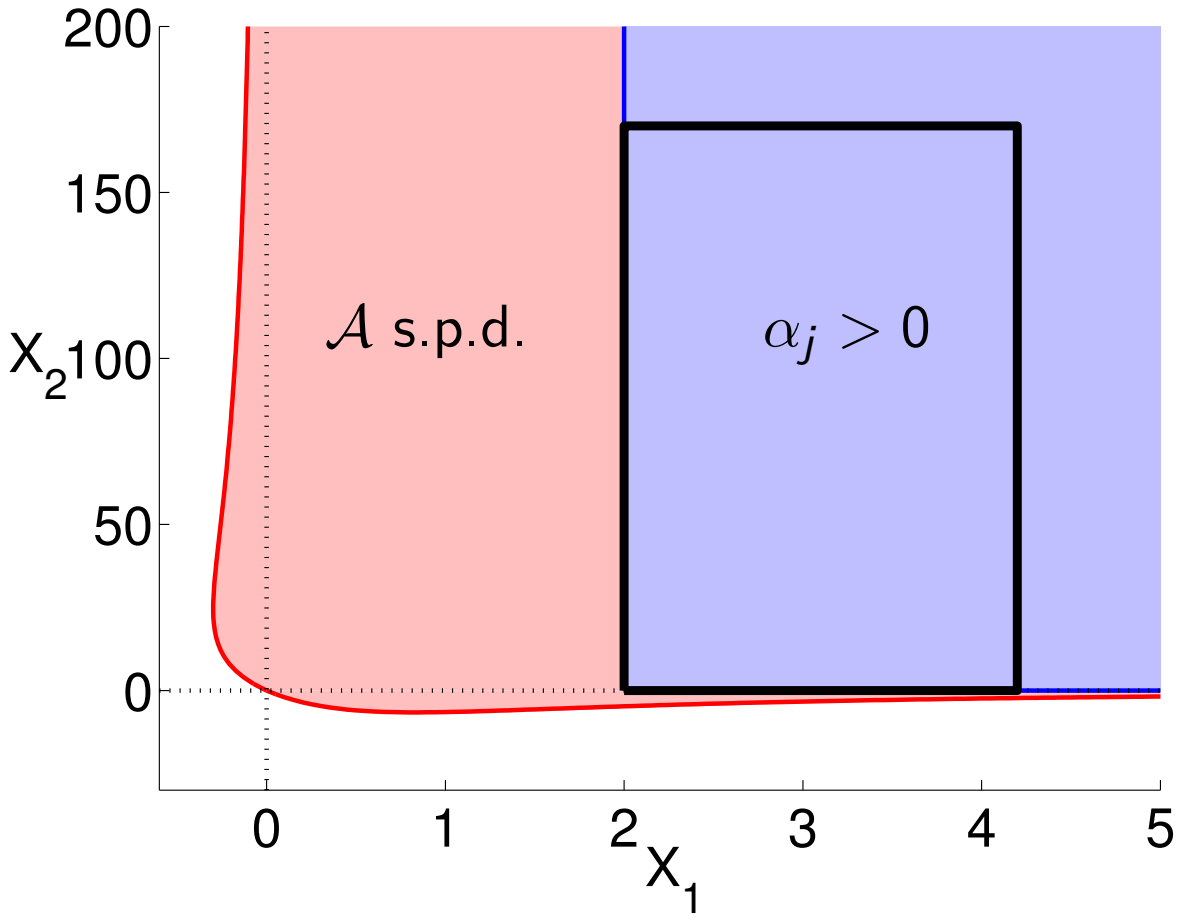

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Time-dependent chemical Fokker-Planck equation

$$\frac{\partial p}{\partial t}(\mathbf{x},t) = \operatorname{div}\left[\operatorname{div}(\mathcal{A}(\mathbf{x})p(\mathbf{x},t)) - \mathbf{b}(\mathbf{x})p(\mathbf{x},t)\right] \quad \text{for } \mathbf{x} \in \Omega,\ t > 0$$

$$0 = \left[\operatorname{div}(\mathcal{A}(\mathbf{x})p(\mathbf{x},t)) - \mathbf{b}(\mathbf{x})p(\mathbf{x},t)\right] \cdot \mathbf{n} \quad \text{for } \mathbf{x} \in \partial\Omega,\ t > 0$$

$$p(\mathbf{x},0) = p_0 \quad \text{for } \mathbf{x} \in \Omega$$

- Choice of Ω?
- No flux boundary conditions $\Rightarrow$ conservativity

Stationary chemical Fokker-Planck equation

$$\begin{aligned} \operatorname{div}\left[\operatorname{div}(\mathcal{A}(\mathbf{x})p(\mathbf{x})) - \mathbf{b}(\mathbf{x})p(\mathbf{x})\right] &= 0 \quad \text{for } \mathbf{x} \in \Omega \\ \left[\operatorname{div}(\mathcal{A}(\mathbf{x})p(\mathbf{x})) - \mathbf{b}(\mathbf{x})p(\mathbf{x})\right] \cdot \mathbf{n} &= 0 \quad \text{for } \mathbf{x} \in \partial\Omega \\ \int_\Omega p(\mathbf{x}) \, \mathrm{d}\mathbf{x} &= 1 \end{aligned}$$

- No flux boundary conditions $\Rightarrow$ 'unique' nontrivial solution based on adjoint problem and Fredholm alternative
- Eigenvalue problem

Zero Dirichlet boundary conditions

Equation:

$$\begin{aligned} \operatorname{div}\left[\operatorname{div}(\mathcal{A}(\mathbf{x})p(\mathbf{x})) - \mathbf{b}(\mathbf{x})p(\mathbf{x})\right] &= 0 \quad \text{for } \mathbf{x} \in \Omega \\ p(\mathbf{x}) &= 0 \quad \text{for } \mathbf{x} \in \partial\Omega \end{aligned}$$

$\Longrightarrow p(\mathbf{x}) = 0$

Eigenvalue problem:

$$\begin{aligned} \operatorname{div}\left[\operatorname{div}(\mathcal{A}(\mathbf{x})p(\mathbf{x})) - \mathbf{b}(\mathbf{x})p(\mathbf{x})\right] &= \lambda_1 p(\mathbf{x}) \quad \text{for } \mathbf{x} \in \Omega \\ p(\mathbf{x}) &= 0 \quad \text{for } \mathbf{x} \in \partial\Omega \end{aligned}$$

$$\int_\Omega p(\mathbf{x})\,\mathrm{d}\mathbf{x} = 1$$

Finite difference method

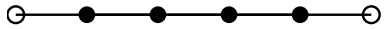
Eigenvalue problem:

$$\begin{aligned} \operatorname{div}\left[\operatorname{div}(\mathcal{A}(\mathbf{x})p(\mathbf{x})) - \mathbf{b}(\mathbf{x})p(\mathbf{x})\right] &= \lambda_1 p(\mathbf{x}) && \text{for } \mathbf{x} \in \Omega \\ p(\mathbf{x}) &= 0 && \text{for } \mathbf{x} \in \partial\Omega \\ \int_\Omega p(\mathbf{x})\,\mathrm{d}\mathbf{x} &= 1 \end{aligned}$$

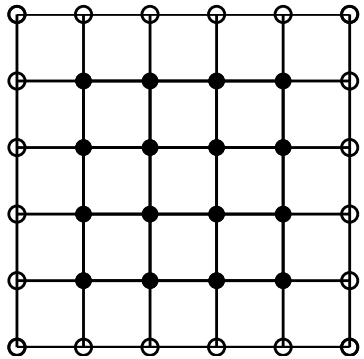
- Cover Ω by a mesh
- Replace derivatives by finite differences
- $\Longrightarrow A\mathbf{p} = \tilde{\lambda}_1 \mathbf{p}$

Curse of dimensionality

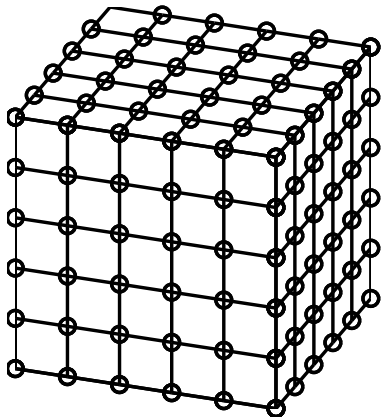
- $N = 1 \Rightarrow n$ nodes



- $N = 2 \Rightarrow n^2$ nodes



- $N = 3 \Rightarrow n^3$ nodes



- In general n^N nodes.

3. Tensor methods

Tensor product of matrices

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \qquad B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$$

$$A \otimes B = \begin{bmatrix} a_{11} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} & a_{12} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} \\ a_{21} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} & a_{22} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{bmatrix}$$

Tensor product of vectors

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$\mathbf{a} \otimes \mathbf{b} = \begin{bmatrix} a_1 \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \\ a_2 \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} a_1 b_1 \\ a_1 b_2 \\ a_1 b_3 \\ a_2 b_1 \\ a_2 b_2 \\ a_2 b_3 \end{bmatrix}$$

$$(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c})_{[ijk]} = a_i b_j c_k$$

Tensor product of vectors

Notice:

$$\mathbf{a}_1 \in \mathbb{R}^n,\ \mathbf{a}_2 \in \mathbb{R}^n,\ \ldots,\ \mathbf{a}_N \in \mathbb{R}^n \quad \Longrightarrow \quad \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \cdots \otimes \mathbf{a}_N \in \mathbb{R}^{n^N}$$

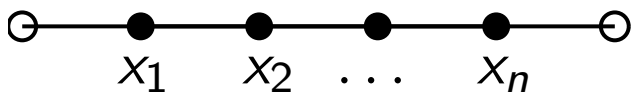
Tensor methods for N dimensional Laplacian

$$
\begin{aligned}
-\Delta u(\mathbf{x}) &= f(\mathbf{x}) \quad && \text{for } \mathbf{x} \in \Omega = (0,1)^N \\
u(\mathbf{x}) &= 0 && \text{for } \mathbf{x} \in \partial\Omega
\end{aligned}
$$

Laplacian in 1D

$$-u''(x) = f(x) \quad \text{for } x \in \Omega = (0,1)$$
$$u(0) = u(1) = 0$$

- x_i form a partition of $(0,1)$



- $i = 1, 2, \ldots, n$
- $\mathbf{f} \in \mathbb{R}^n$, $\mathbf{f}_i = f(x_i)$
- $\mathbf{u} \in \mathbb{R}^n$, $u(x_i) \approx u_i$
- $-u''(x_i) \approx \dfrac{-u_{i-1} + 2u_i - u_{i+1}}{h^2}$
- $-u''(x) \approx D\mathbf{u}$
- $D\mathbf{u} = \mathbf{f}$

$$D = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 2 \end{bmatrix}$$

Laplacian in 2D

$$-\frac{\partial^2 u}{\partial x_1^2}(x_1, x_2) - \frac{\partial^2 u}{\partial x_2^2}(x_1, x_2) = f(x_1, x_2) \quad \text{for } (x_1, x_2) \in \Omega = (0,1)^2$$

$$u(x_1, x_2) = 0 \quad \text{for } \mathbf{x} \in \partial\Omega$$

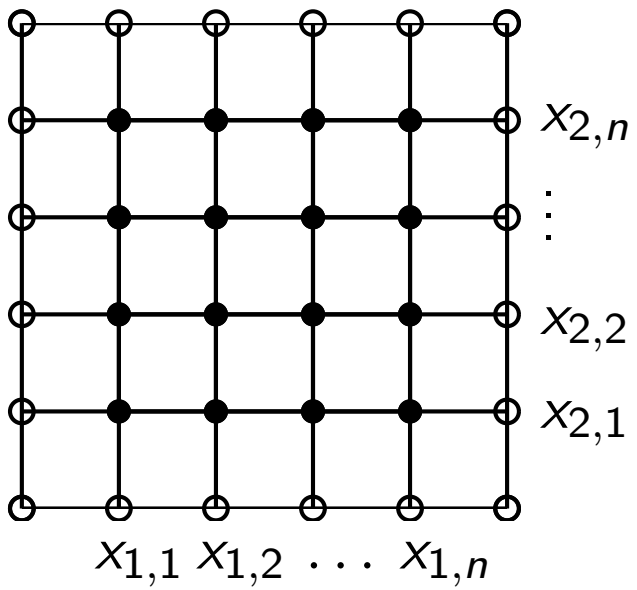
If $u(x_1, x_2) = q_1(x_1)q_2(x_2)$ then

$$-\Delta u(x_1, x_2) = -q_1''(x_1)q_2(x_2) - q_1(x_1)q_2''(x_2)$$

$$-\Delta u \approx (D\mathbf{q}_1) \otimes \mathbf{q}_2 + \mathbf{q}_1 \otimes (D\mathbf{q}_2)$$

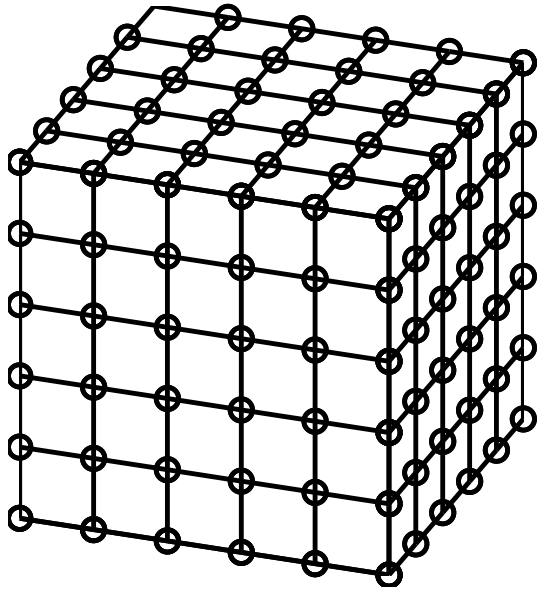
$$= \underbrace{(D \otimes I + I \otimes D)}_{A} \underbrace{(\mathbf{q}_1 \otimes \mathbf{q}_2)}_{\mathbf{u}}$$

$\Longrightarrow A\mathbf{u} = \mathbf{f}$



Laplacian in 3D

- $A = D \otimes I \otimes I + I \otimes D \otimes I + I \otimes I \otimes D$
- $A\mathbf{u} = \mathbf{f}$



$$u(x_1, x_2, x_3) \approx \sum_{r=1}^{R} q_1^r(x_1) q_2^r(x_2) q_3^r(x_3)$$

$$\mathbf{u} \approx \sum_{r=1}^{R} \mathbf{q}_1^r \otimes \mathbf{q}_2^r \otimes \mathbf{q}_3^r$$

$$A\mathbf{u} = (D \otimes I \otimes I + I \otimes D \otimes I + I \otimes I \otimes D) \left(\sum_{r=1}^{R} \mathbf{q}_1^r \otimes \mathbf{q}_2^r \otimes \mathbf{q}_3^r \right)$$

$$= \sum_{r=1}^{R} (D\mathbf{q}_1^r) \otimes \mathbf{q}_2^r \otimes \mathbf{q}_3^r + \mathbf{q}_1^r \otimes (D\mathbf{q}_2^r) \otimes \mathbf{q}_3^r + \mathbf{q}_1^r \otimes \mathbf{q}_2^r \otimes (D\mathbf{q}_3^r)$$

Tensor format

Tensor truncation:

$$\sum_{r=1}^{R} \mathbf{q}_1^r \otimes \mathbf{q}_2^r \otimes \cdots \otimes \mathbf{q}_N^r \approx \sum_{s=1}^{S} \mathbf{v}_1^s \otimes \mathbf{v}_2^s \otimes \cdots \otimes \mathbf{v}_N^s \quad \text{with } S < R$$

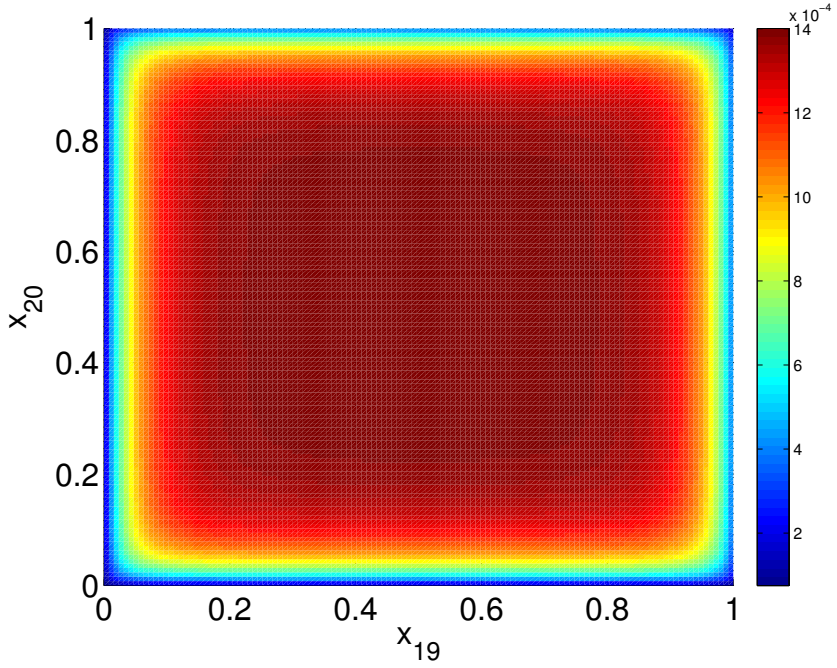
Canonical decomposition:

$$\mathbf{u} \approx \underbrace{\sum_{r=1}^{R} \mathbf{q}_1^r \otimes \mathbf{q}_2^r \otimes \cdots \otimes \mathbf{q}_N^r}_{nNR \text{ entries}}, \quad \text{where } \mathbf{q}_d^r \in \mathbb{R}^n, d = 1, 2, \ldots, N$$

Numerical stability $\Rightarrow$ Tensor train format

Example: 20D Laplacian

$$-\Delta u(\mathbf{x}) = 1 \quad \text{for } \mathbf{x} \in \Omega = (0,1)^{20}$$
$$u(\mathbf{x}) = 0 \quad \text{for } \mathbf{x} \in \partial\Omega$$



Plot of $\tilde{u}(x_{19}, x_{20}) = \int_0^1 \cdots \int_0^1 u(x_1, \ldots, x_{20})\, \mathrm{d}x_1 \cdots \mathrm{d}x_{18}$

Chemical Fokker-Planck equation

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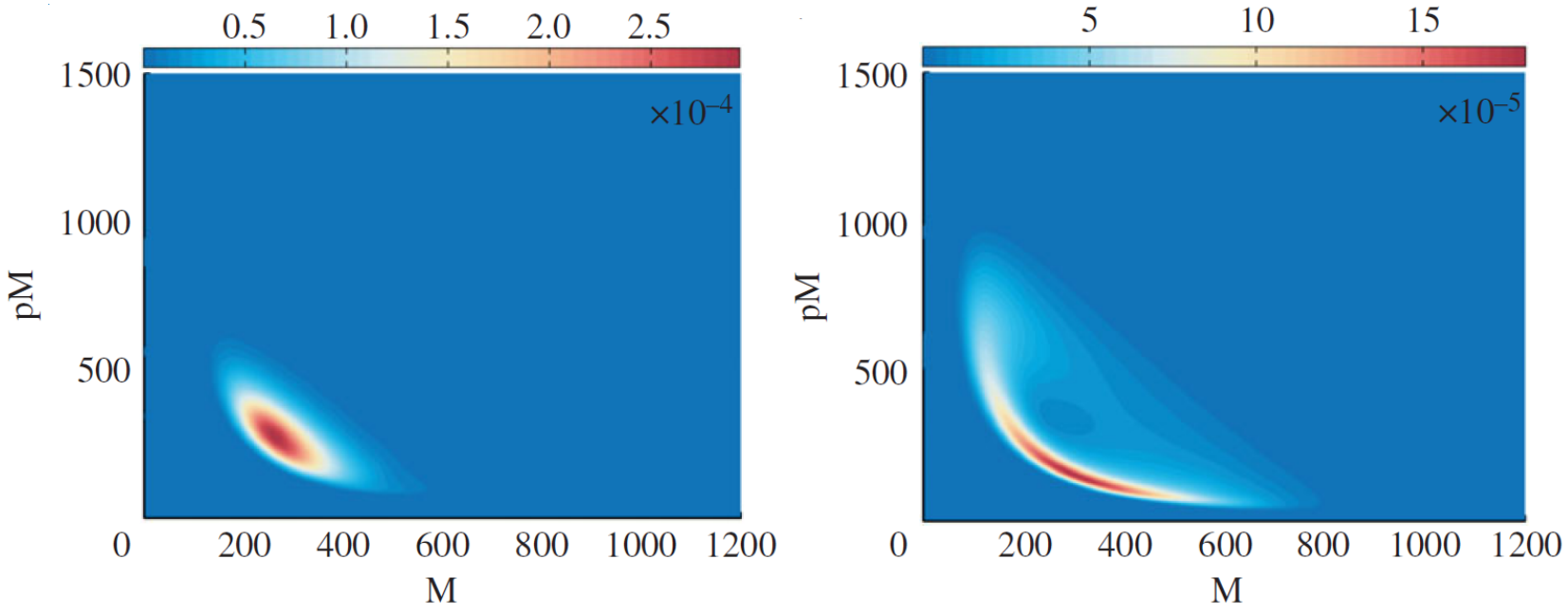
- $\mathcal{A}_{ik}(\mathbf{x}) = \frac{1}{2}\sum_{j=1}^{M} \nu_{ji}\nu_{jk}k_j \prod_{i=1}^{N} \binom{x_i}{\nu_{ji}^{\mathrm{r}}}$
- $b_i(\mathbf{x}) = \sum_{j=1}^{M} \nu_{ji}k_j \prod_{i=1}^{N} \binom{x_i}{\nu_{ji}^{\mathrm{r}}} \quad \Longrightarrow \quad A\mathbf{p} = \tilde{\lambda}_1\mathbf{p}$
- TT-toolbox by Ivan Oseledets et al.
- Unknown parameter as an additional dimension
- Multilevel approach

Bifurcation analysis of the stochastic cell cycle model



- 6 chemical species + 1 parameter dimension
- [S. Liao, T. Vejchodsky, R. Erban: J. R. Soc. Interface 12 (108), 2015, 20150233]

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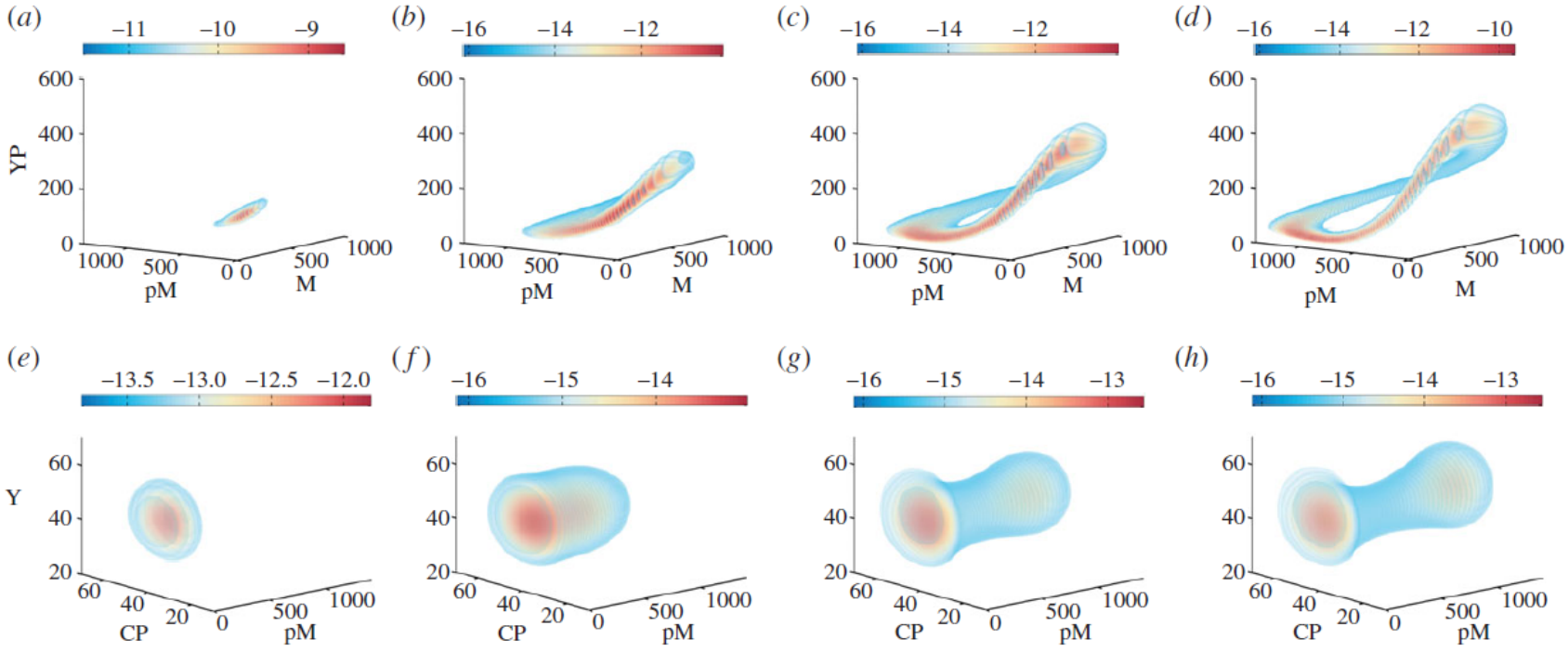

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4. Error estimation

Type of errors

- Error of Fokker-Planck equation
- Error caused by the domain truncation
- Error of artificial boundary conditions
- Discretization error
- Tensor error
- Algebraic error

Future work:

- estimates of individual errors
- equilibrate individual errors

Conclusion

- Tensor methods can break the curse of dimensionality.
- Parametric chemical Fokker-Planck equation
  - Bifurcation analysis
  - Parameter estimation
  - Sensitivity analysis
- Tensor methods can be combined with the FEM, DG, etc.
- Tensor methods can solve the chemical master equation.

Thank you for your attention

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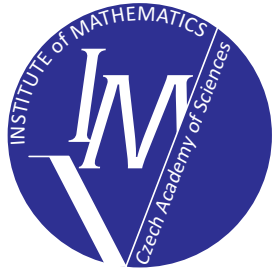

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