WESTFÄLISCHE WILHELMS-UNIVERSITÄT MÜNSTER

APPLIED MATHEMATICS MÜNSTER

Model reduction for kinetic transport equations

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M. Ohlberger K. Smetana

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Motivation

Example: Radiotherapy

$\Downarrow$

Transport equations for Electrons and Photons

$\underbrace{\qquad\qquad\qquad}$

kinetic equations

- describe the density of particles in phase space, usually consisting of
  - d spatial variables
  - d momentum or velocity variables
- time-dependent problem $\Longrightarrow$ $(2d+1)$-dimensional computational domain

$\Longrightarrow$ (Dimensional) model reduction can be beneficial

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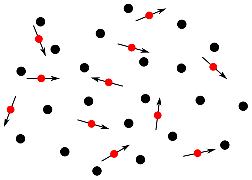

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Outline

Fokker-Planck equation

Hierarchical Model Reduction

Problem adapted basis functions
- Parametrized PDE in the velocity variable
- Basis generation with Reduced Basis techniques

Numerical Experiments

Outlook

Fokker-Planck equation

Consider the 1D Fokker-Planck (FP) equation[1]:

$$\partial_t \psi(t,x,v) + v \partial_x \psi(t,x,v) = T(t,x) \partial_v \left((1 - v^2) \partial_v \psi(t,x,v) \right)$$

for $t \in [0, t_1]$, $x \in (a, b)$, $v \in (-1, 1)$.

- $T(t,x)$: "Transport Coefficient" depending on scattering kernel
- Additional source and reaction terms left out for convenience
- Ingoing radiation at the spatial boundary:

$$\psi(t,a,v) = \psi_a(t,v) \text{ for } v > 0, \quad \psi(t,b,v) = \psi_b(t,v) \text{ for } v < 0,$$

- Initial condition: $\psi(0,x,v) = \psi_0(x,v)$.

[1]for this form see [Schneider, Alldredge, Frank, Klar 2014]

Existing dimensional reduction approaches

- Method of Moments
  - [Frank, Hensel, Klar 2007]
  - [Schneider, Alldredge, Frank, Klar 2014]
  - [Klar, Schneider, Tse 2014]
  - ...
- Sparse Tensor Approximation
  - [Widmer, Hiptmaier, Schwab 2008]
  - [Grella, Schwab 2011]
  - ...
- Proper Generalized Decomposition
  - [Ammar, Mokdad, Chinesta, Keunings 2006/07]
  - [Chinesta, Abisset-Chavanne, Ammar, Cueto 2015]
  - ...
- ...

Hierarchical Model Reduction

Ansatz:

$$\psi(t,x,v) = \sum_{i=1}^{m} \hat{\psi}_i(t,x)\phi_i(v)$$

1. Choose *basis of the reduced velocity space*:

$$\phi_i(v),\ i = 1,\dots,m \quad (L^2\text{-orthogonal})$$

2. Solve problem for $\hat{\psi}_i(t,x)$, $i = 1,\dots,m$, with fixed $\phi_i(v)$

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Derivation of the reduced system for $\widehat{\psi}_i(t,x)$

Fokker-Planck equation:

$$\partial_t \psi(t,x,v) + v\partial_x \psi(t,x,v) = T(t,x)\partial_v \left((1-v^2)\partial_v \psi(t,x,v)\right),$$

- Assume $\phi_i(v)$, $i = 1,\dots,m$ to be given.
- Insert ansatz
- Test with $\phi_k(v)$, $k = 1,\dots,m$, (define $(f_1,f_2)_V := \int_{-1}^{1} f_1(v) f_2(v) \mathrm{d}v$)
- Set $\widehat{\psi}(x,t) = (\widehat{\psi}_1(t,x),\dots,\widehat{\psi}_m(t,x))^T$ and write as linear system

Derivation of the reduced system for $\widehat{\psi}_i(t,x)$

$$\partial_t\left(\sum_{i=1}^{m}\widehat{\psi}_i(t,x)\phi_i(v)\right)+v\partial_x\left(\sum_{i=1}^{m}\widehat{\psi}_i(t,x)\phi_i(v)\right)$$
$$=T(t,x)\partial_v\left((1-v^2)\partial_v\left(\sum_{i=1}^{m}\widehat{\psi}_i(t,x)\phi_i(v)\right)\right).$$

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Derivation of the reduced system for $\widehat{\psi}_i(t,x)$

$$\sum_{i=1}^{m}(\phi_i(v),\phi_k(v))_v\partial_t\widehat{\psi}_i(t,x)+\sum_{i=1}^{m}(v\phi_i(v),\phi_k(v))_v\partial_x\widehat{\psi}_i(t,x)$$
$$=-\sum_{i=1}^{m}\left((1-v^2)\partial_v\phi_i(v),\partial_v\phi_k(v)\right)_v T(t,x)\widehat{\psi}_i(t,x)$$
$$\forall\, k=1,\dots,m.$$

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Derivation of the reduced system for $\widehat{\psi}(t,x)$

$$\boldsymbol{M}\partial_t\widehat{\psi}(x,t) + \boldsymbol{D}\partial_x\widehat{\psi}(x,t) + T(t,x)\boldsymbol{S}\widehat{\psi}(x,t) = 0$$

with

$$\begin{aligned}
\boldsymbol{M} &= (M_{ij}) \in \mathbb{R}^{m\times m}, \quad & M_{ji} &:= (\phi_i(v), \phi_j(v))_v,\\
\boldsymbol{D} &= (D_{ij}) \in \mathbb{R}^{m\times m}, \quad & D_{ji} &:= (v\phi_i(v), \phi_j(v))_v,\\
\boldsymbol{S} &= (S_{ij}) \in \mathbb{R}^{m\times m}, \quad & S_{ji} &:= \big((1-v^2)\partial_v\phi_i(v), \partial_v\phi_j(v)\big)_v,
\end{aligned}$$

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- Set $\widehat{\psi}(x,t) = (\widehat{\psi}_1(t,x),\dots,\widehat{\psi}_m(t,x))^T$ and write as linear system

Choice of basis functions $\phi_i(v)$

Existing methods: Choice of $\phi_i(v)$ **a priori** (e.g. monomials or Legendre polynomials $\rightarrow$ *Method of Moments*)

Aim: Choice of $\phi_i(v)$ adapted to the considered problem

Idea: ([Ohlberger, Smetana 14], [Smetana, Ohlberger, 17][2])

- Derive a parametrized PDE solely in v-direction
  - unknown behavior of solution in x- and t-direction contained as parameters
- Generate $\phi_i(v)$ from solutions of this PDE (so-called snapshots)
  - use Reduced Basis[3] techniques

[2] developed an HMR-RB approach for two-dimensional elliptic equations and nonlinear PDEs

[3] Introduction: [Quarteroni, Manzoni, Negri 2016]

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Derivation of parametrized problem in v-direction[1]

- Assume that the solution can be written as

$$\psi(t,x,v) \approx \underbrace{\mathcal{U}(t,x)}_{\text{unknown behavior of the full solution in } x \text{ and } t} \phi(v),$$

- Test FP equation with $\mathcal{U}(t,x)\varphi(v)$ for $\varphi \in H_0^1((-1,1))$:

$$(\partial_t \mathcal{U}(t,x), \mathcal{U}(t,x))_{t,x}(\phi(v),\varphi(v))_v + (\partial_x \mathcal{U}(t,x), \mathcal{U}(t,x))_{t,x}(v\phi(v),\varphi(v))_v$$
$$= -(T(t,x)\mathcal{U}(t,x), \mathcal{U}(t,x))_{t,x}((1-v^2)\partial_v\phi(v), \partial_v\varphi(v))_v,$$

where $\int_0^{t_1}\int_a^b f_1(t,x) f_2(t,x)\,\mathrm{d}x\mathrm{d}t =: (f_1,f_2)_{t,x}$.

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- $\mathcal{U}(t,x)$ unknown $\rightarrow$ Integrals cannot be precomputed
- Introduce quadrature formula for the integrals:

$$(u_1,u_2)_{t,x} = \int_0^{t_1}\int_a^b u_1(t,x)u_2(t,x)\mathrm{d}x\mathrm{d}t$$
$$\approx \sum_{q=1}^{\tilde{q}} \omega_q u_1(t^q,x^q)u_2(t^q,x^q) =: (u_1,u_2)_{t,x}^q,$$

ω_q, $q=1,\dots,\tilde{q}$, weights, (t^q,x^q), $q=1,\dots,\tilde{q}$, quadrature points

Parameter

Define parameter containing

- Quadrature points $(t^q, x^q)_{1 \leqslant q \leqslant \tilde{q}}$
- Needed values of $\mathcal{U}$, $\partial_x \mathcal{U}$, $\partial_t \mathcal{U}$ at the quadrature points

Parameter:

$$\mu = \Big((t^q, x^q)_{1 \leqslant q \leqslant \tilde{q}}, \big(\mathcal{U}(t^q, x^q) \big)_{1 \leqslant q \leqslant \tilde{q}}, \big(\partial_x \mathcal{U}(t^q, x^q) \big)_{1 \leqslant q \leqslant \tilde{q}}, \big(\partial_t \mathcal{U}(t^q, x^q) \big)_{1 \leqslant q \leqslant \tilde{q}} \Big).$$

Parameter space: $\mathcal{D} := [0, t_1]^{\tilde{q}} \times [a, b]^{\tilde{q}} \times I_0^{\tilde{q}} \times I_1^{\tilde{q}} \times I_2^{\tilde{q}} \subset \mathbb{R}^P$.

- I_0, I_1, and I_2 contain ranges of $\mathcal{U}$, $\partial_x \mathcal{U}$, $\partial_t \mathcal{U}$,.

$\Longrightarrow$ Parameter includes information on the unknown behavior $\mathcal{U}$ in x- and t- direction

$\Longrightarrow$ Good locations of quadrature points can be found with Reduced Basis techniques

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Parametrized problem in v-direction

- Define lifting function $\phi_b(v)$ for non-homogeneous Dirichlet B.C.

Given any $\mu \in \mathcal{D}$, find $\phi \in H^1((-1,1))$ such that $\phi - \phi_b \in H^1_0((-1,1))$ and

$$a(\mu)\left((1-v^2)\partial_v\phi(v), \partial_v\varphi(v)\right)_v + b(\mu)(v\phi(v), \varphi(v))_v + c(\mu)(\phi(v), \varphi(v))_v = 0 \quad \forall \varphi \in H^1_0((-1,1)),$$

where $a(\mu) := (T\mathcal{U}, \mathcal{U})^q_{t,x}$,

$b(\mu) := (\partial_x\mathcal{U}, \mathcal{U})^q_{t,x}$,

$c(\mu) := (\partial_t\mathcal{U}, \mathcal{U})^q_{t,x}$.

Reduced Basis Method

Detailed introduction: e.g. [Quarteroni, Manzoni, Negri 2016],
Transport problems: [Dahmen, Huang, Schwab, Welper 2012], [Dahmen, Plesken, Welper 2014]

- Model reduction technique for parametrized PDEs
- Setting: PDE needs to be solved for a large number of parameter values

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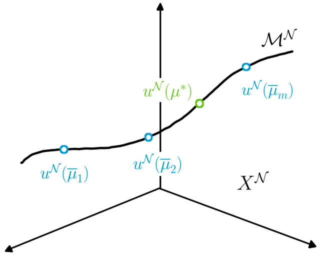
- Key idea: dim(Solution Manifold) $\ll$ dim(Solution Space)



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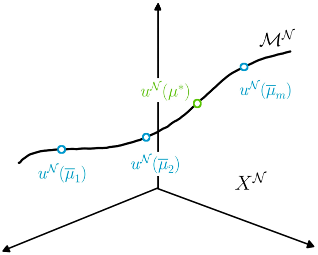
- Key idea: dim(Solution Manifold) $\ll$ dim(Solution Space)

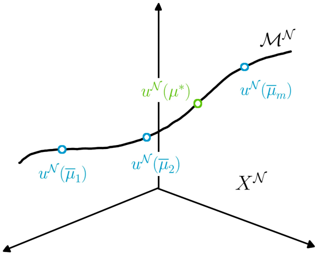
$\Longrightarrow$ Find low-dimensional reduced space that resembles the solution manifold



Reduced Basis Method

To find the reduced space:

- Compute so-called snapshots, i.e. solutions of the PDE for certain particular parameter values
- Choose reduced space as (subspace of) span of these snapshots



Different possibilities

- How to choose parameter values for the snapshots
- How to determine the Reduced Basis, i.e. the basis of the reduced space

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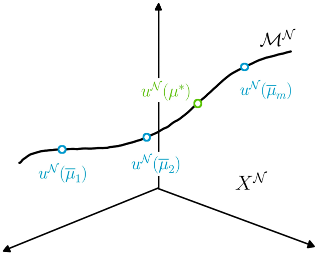

Different possibilities

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Reduced Basis Method

Basis generation algorithms:

Proper Orthogonal Decomposition (POD):

- Compute solutions $\mathcal{P}^h(\mu)$ of the parametrized PDE for all parameter values μ from a *training set* Ξ (e.g. random parameter values)
- Define the POD space of order k as the best approximation space

$$Y_k^{POD} := \operatorname{arginf}_{W_k \subset \mathrm{Span}\{\mathcal{M}^h_\Xi\}} \left(\frac{1}{n_{train}} \sum_{\mu \in \Xi} \inf_{w_k \in W_k} \left\| \mathcal{P}^h(\mu) - w_k \right\|^2_{L^2(\omega)} \right).$$

- Can be computed by a singular value decomposition (SVD) of the matrix of all snapshots

Reduced Basis Method

Basis generation algorithms:

Greedy Algorithm

- Iteratively:
  - Compute reduced solutions for the current reduced basis for all parameter values in the *training set*.
  - Calculate or estimate the model errors for all parameter values
  - Choose the snapshot of the parameter value with the largest error, i.e. the worst approximation to extend the basis

$\Longrightarrow$ **Aim:** Good approximation properties for the whole training set

- Minimizes maximal error of all parameters
- Algorithm can produce rate-optimal reduced spaces, i.e. near-optimal approximation spaces, see [DeVore, Petrova, Wojtaszczyk 2013]

Hierarchical Model Reduction

Setting:

- Problem: High-dimensional Fokker-Planck equation
- Nonlinear approximation by basis expansion in velocity variable
- Parametrized PDE in v to generate functions that represent velocity dependence of solution
- Error of reduced solution to FP equation should be low

Aim:

- Fit RB basis generation algorithm to our setting

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HMR Basis Generation

Greedy:

Iterately

- Compare errors of reduced solutions with different velocity basis to high-dimensional solution
- Choose snapshot that leads to best reduced solution as new basis function

  $\Longrightarrow$ Basis chosen to generate one reduced solution as good as possible

HMR Greedy Algorithm

Algorithm 1: GreedyBasisGeneration

Data: $\Xi = \{\phi^n : n = 1, \ldots, n_{\text{sample}}\}, h_x, m_{\text{max}}$

Initialize $\Phi_0 = \emptyset$;

for $m = 1 : m_{max}$ **do**

  for $n = 1 : n_{sample}$ **do**

    $\tilde{\Phi}^n := \text{GramSchmidtProcess}(\Phi_{m-1} \cup \{\phi^n\})$;

    if $\dim(\tilde{\Phi}^n) = m$ **then**

      $\psi^n := \text{SolveFPSystem}(\tilde{\Phi}^n, h_x)$;

      $e_n := \text{L1Error}(\psi^n)$;

    end

  end

  $\tilde{n} := \text{argmin}_n(e_n)$;

  $\Phi_m := \tilde{\Phi}^{\tilde{n}}$;

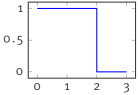
end

Numerical Experiments

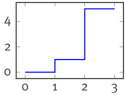
Model Problem: SourceBeam test case[2]

We consider a domain $x \in (0,3)$ in time $t \in [0,4]$. Full FP equation:

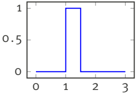
$$\partial_t\psi + v\partial_x\psi + \underbrace{\sigma_a\psi} = \underbrace{T}\,\partial_v\left((1-v^2)\partial_v\psi\right) + \underbrace{Q},$$



Reaction term $\sigma_a(x)$

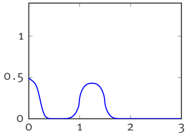


Transport coeff. $T(x)$

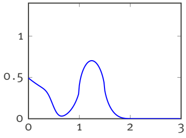


Source $Q(x)$

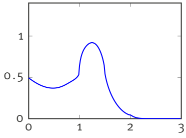
I.C. and B.C.: $\psi_0 = 0, \quad \psi_l(v>0) = \delta(v-1), \quad \psi_r = 0$



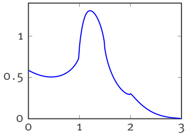
$t = 0.25$



$t = 0.5$



$t = 1$



$t = 4$

[2] (from [Schneider, Alldredge, Frank, Klar 2014])

HMR with “truth-snapshots”

- $\psi^{\text{ref}}(t, x, v)$ full-dimensional reference solution
- Define “truth-snapshots” for points (t_i, x_i): $s_i(v) := \psi^{\text{ref}}(t_i, x_i, v)$.
- Snapshot set: 192 “truth-snapshots” for (x_i, t_i) on coarse rectangular grid of size 12×16

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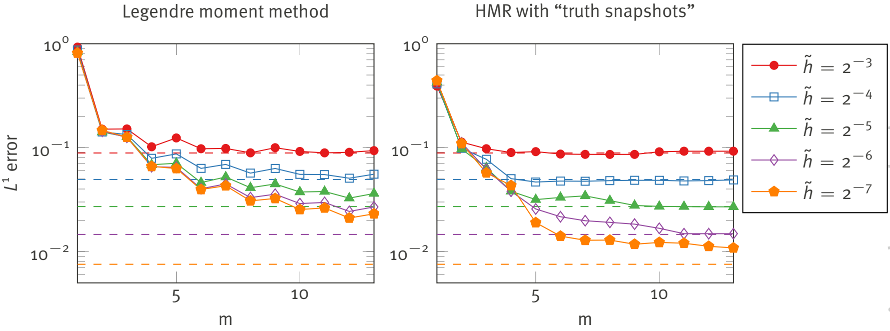

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- Use one quadrature point (t^1, x^1)
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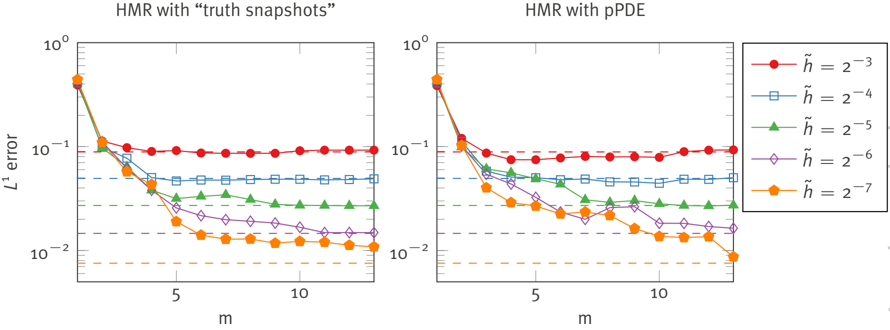

Summary

- Hierarchical model reduction approach for the Fokker-Planck equation
- (Truncated) basis expansion in the velocity variable
- Parametrized PDE in the velocity variable, parameters reflect unknown behavior of the solution in space and time variables
- Basis generation by a greedy algorithm inspired by RB methods
- Numerical Experiments:
  - Good convergence behavior, better than a priori chosen Legendre polynomials
  - Drawback: Basis generation very expensive, performance has to be improved

Outlook

Ongoing work:

- Space-time variational formulations for time-dependent transport equations

Advantage:

- (Full) discretized solutions and reduced solutions can be defined as Petrov-Galerkin projections
- (Efficient) a posteriori error estimation possible

Next steps / future work:

- New HMR ansatz
  - Use different trial and test spaces
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Thank you for your attention!

J. Brunken, T. Leibner, M. Ohlberger, and K. Smetana.
Problem adapted hierarchical model reduction for the Fokker-Planck equation.
In *Proceedings of ALGORITMY 2016, 20th Conference on Scientific Computing, Vysoke Tatry, Podbanske, Slovakia, March 13-18, 2016*

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http://wwwmath.uni-muenster.de/num/ohlberger/

Spatial density, considered errors

We always consider the spatial density

$$\psi^{(0)}(t,x) := \int_{-1}^{1} \psi(t,x,v)\mathrm{d}v$$

of the solutions.

In all numerical tests we compare two solutions by computing the relative L^1-error between the respective spatial densities:

$$e_{L^1}(\psi_1(t,x,v),\psi_2(t,x,v)) := \frac{\int_a^b \int_0^{t_1} |\psi_1^{(0)}(t,x) - \psi_2^{(0)}(t,x)|\mathrm{d}t\mathrm{d}x}{\int_a^b \int_0^{t_1} |\psi_1^{(0)}(t,x)|\mathrm{d}t\mathrm{d}x}.$$

Outlook - Variational Formulation

Ongoing (joint work with K. Smetana and K. Urban):

- Derivation of stable space-time variational formulations for (general) time-dependent transport equations
- Problem: Define spatial operator $A : H \to V'$, then find u such that

$$\dot{u}(t) + Au(t) = g(t) \quad \text{in } V', t \in I,$$
$$u(0) = 0 \quad \text{in } V'.$$

- Use variational formulation based on bilinear form

$$b(v,w) := \int_0^T \langle \dot{v}(t), w(t) \rangle_{V' \times V} dt + \int_0^T a(v(t), w(t)) dt$$

with trial space $\mathcal{X} := L^2(I;H) \cap H^1_{(0)}(I;V')$ and test space $\mathcal{Y} = L^2(I;V)$