Contributions for the approximation and model order reduction of partial differential equations

Habilitation à diriger des recherches

Marie Billaud-Friess

Centrale Nantes, Nantes Université
Laboratoire Mathématiques Jean Leray

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We seek $\mathsf{u}(\xi) : y \mapsto \mathsf{u}(y,\xi)$, depending on (random) parameter $\xi \in \Xi \subset \mathbb{R}^p$, solution of

$$\mathcal{P}(\mathsf{u}(\xi),\xi) = 0,$$

with $\mathcal{P}$ some parameter-dependent partial differential operator.

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Forward problems related to parameter-dependent PDEs.

✓ Usual discretization methods provide a numerical solution in vector space V

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Model order reduction approaches. Approximation methods providing a surrogate u_r of

$$u : \Xi \to V,$$

that can be evaluated for any $\xi \in \Xi$ at low complexity.

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- How to deal with high dimensional problems ?

1. Time independent linear problems
2. Time dependent non-linear problems
3. Conclusion

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PhD O. Zahm : (B.-F., Nouy, Zahm,2013) (B.-F., Nouy, Zahm,2014) (Zahm, B.-F., Nouy,2017)

PhD A. Macherey: (B.-F., Macherey, Nouy, Prieur,2020) (B.-F., Macherey, Nouy, Prieur,2022) (B.-F., Macherey, Nouy, Prieur,in preparation)

Let $D \subset \mathbb{R}^d$ be an open bounded domain with boundary ∂D and $\Xi \subset \mathbb{R}^p$ be a parameter set. We seek, for all $\xi \in \Xi$, $\mathsf{u}(\xi) : D \to \mathbb{R}$ solution of

$$\begin{array}{rcll} -\mathcal{A}(\xi)\mathsf{u}(\xi) & = & \mathsf{g}(\xi), & \text{in } D, \\ \mathsf{u}(\xi) & = & \mathsf{f}(\xi), & \text{on } \partial D, \end{array} \quad (1)$$

with given functions $\mathsf{g} : \bar{D} \times \Xi \to \mathbb{R}$ and $\mathsf{f} : \partial D \times \Xi \to \mathbb{R}$.

Here $\mathcal{A}(\xi)$ stands for the following partial differential operator

$$\mathcal{A}(\xi) = \frac{1}{2} \sum_{i,j=1}^{d} (\sigma(\xi)\sigma(\xi)^T)_{ij} \partial^2_{x_i x_j} + \sum_{i=1}^{d} b_i(\xi) \partial_{x_i} - k(\xi),$$

with $b(\xi) : \mathbb{R}^d \times \Xi \to \mathbb{R}^d$, $\sigma(\xi) : \mathbb{R}^d \to \mathbb{R}^{d \times d}$ and $k(\xi) : \mathbb{R}^d \to \mathbb{R}^*_+$.

Low-rank approximation for parameter-dependent problems in nutshell

We want to approximate $u : \Xi \to V$ with V some high dimensional vector space.

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Linear approximation.

We seek u_r as the rank-r approximation of $u \in X := V \otimes S$

$$u_r(\xi) = \sum_{i=1}^{r} \alpha_i(\xi) v_i$$

with $\{v_1, \dots, v_r\} \subset V$ and $\{\alpha_1, \dots, \alpha_r\} \subset S$ a vector space of functions defined on Ξ.

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Two points of view. (Nouy,2017)

① Approximation in low-rank tensor subset $\mathcal{M}_r(X)$ of X

② Low-rank approximation methods based on projection in subspace V_r of V

① Approximation in low-rank tensor subset: with greedy algorithm

Let X (sim. Y) be Hilbert tensor space with dual X' and $A \in \mathcal{L}(X, Y')$.

Here, $u \in X$ is solution of

$$Au = b, \text{ in } Y'. \tag{2}$$

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Tensor subset. For $X = V \otimes S$, we define the low-rank tensor subset

$$\mathcal{M}_r(X) = \left\{ v = \sum_{i=1}^{r} \alpha_i(\xi) v_i : v_i \in V, \alpha_i \in S \right\}.$$

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Other suitable tensor formats are also possible (Hackbush, 2012).

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Minimal residual approximation. We seek $u_r \approx u$ as

$$u_r \in \underset{v \in \mathcal{M}_r(X)}{\arg\min} \|Av - b\|_{Y'}. \tag{3}$$

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Greedy computation of u_r.

For $r \geq 1$, compute $u_r = u_{r-1} + w_r$ with

$$w_r \in \arg\min_{w \in \mathcal{M}_1(X)} \|A(u_{r-1} + w) - b\|_{Y'}.$$

Ideal minimal residual method (B.-F., Nouy, Zahm,2013) (B.-F., Nouy, Zahm,2014)

The approximation $u_r \in \mathcal{M}_r(X)$ is sought as

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Ideal norm. If we choose (Cohen, Dahmen, Welper,2012) (Dahmen, Huang, Schwab, Welper,2012)

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Practical approach. Perturbated gradient type algorithm

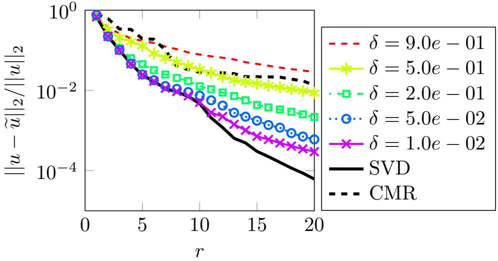
1. Compute an approximation of the residual with prescribed precision δ.
2. Compute a quasi-optimal approximation of the update (using greedy procedure).

$\Rightarrow$ The algorithm converges towards a neighborhood of the best approximation.

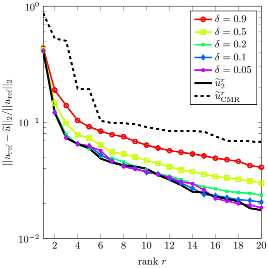
Confronted approaches.

1. Black : Reference solution
2. Dashed black: Minimal residual with canonical norm
3. Perturbated ideal minimal residual with precision δ

Small dimension $p = 1$



High dimension $p = 9$



Relative approximation error in canonical norm with respect to rank.

② Projection based approach : reduced basis method (RBM)

Let V (sim. W) be Hilbert space and $A(\xi) \in \mathcal{L}(V, W')$.

For all $\xi \in \Xi$, we seek $u_r(\xi) \approx u(\xi) \in V$ solution of

$$A(\xi)u(\xi) = b(\xi), \quad \xi \in \Xi \tag{6}$$

in a low-dimensional subspace $V_r \subset V$ with $\dim(V_r) = r$.

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Offline : greedy construction of V_r.

Let $\tilde{\Xi} \subset \Xi$ be a discrete training set and $V_0 = \{0\}$. For $r \geq 1$ proceed as follows.

1) Select

$$\xi_r \in \arg\max_{\xi \in \tilde{\Xi}} \Delta(u_{r-1}(\xi), \xi).$$

2) Compute the snapshot $u(\xi_r)$ and update $V_r = \text{span}\{u(\xi_1), \ldots, u(\xi_r)\}$.

$\Delta(u_r(\xi), \xi)$ is a suitable error estimate computable from the equation residual.

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Online: computation of $u_r(\xi)$. It is obtained from suitable projection in V_r using the equation residual, with complexity depending only on r.

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But what if, we have access to pointwise estimates of $\mathsf{u}(x, \xi)$ for any $(x, \xi) \in D \times \Xi$?

The partial operator

$$\mathcal{A}(\xi) = \frac{1}{2}\sum_{i,j=1}^{d}(\sigma(\xi)\sigma(\xi)^T)_{ij}\partial^2_{x_i x_j} + \sum_{i=1}^{d} b_i(\xi)\partial_{x_i},$$

is the infinitesimal generator related to the diffusion process $X^{x,\xi}$ solution of

$$dX_t^{x,\xi} = b(X_t^{x,\xi},\xi)dt + \sigma(X_t^{x,\xi},\xi)\; dW_t \quad t \geq 0, \tag{7}$$

starting from $X_0^{x,\xi} = x \in \overline{D}$ with W a d-dimensional brownian motion on $(\Omega, \mathcal{F}, \mathbb{P})$.

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Probabilistic representation. By Feynman-Kac (FK) formula, for all $x \in \overline{D}$ we have

$$\mathsf{u}(x,\xi) = \mathbb{E}\left(\mathsf{f}(X_{\tau^{x,\xi}}^{x,\xi},\xi) + \int_0^{\tau^{x,\xi}} \mathsf{g}(X_t^{x,\xi},\xi)dt\right), \tag{8}$$

where $X^{x,\xi}$ is solution of (7) stopped at $t = \tau^{x,\xi}$. (Friedman [§6,Theorem 2.4],2010)

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$\Rightarrow$ Monte-Carlo estimates of $\mathsf{u}(x,\xi)$

Sample based projection.

Using FK samples, we compute snapshots $u(\xi)$ and $u_r(\xi)$ avoiding the equation residual.

$\Rightarrow$ Least-square methods

$\Rightarrow$ Interpolation (within control variate setting and $d >> 1$)

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Probabilistic interpretation of the square norm of the current error.

We choose

$$\Delta(u_r(\xi),\xi) = \|\mathrm{u}(\xi) - u_r(\xi)\|^2_{L^2(D)} = \mathbb{E}\left(Z_r(\xi)\right),$$

where $Z_r(\xi)$ are computed from FK samples of $\mathrm{u}(\xi) - u_r(\xi)$.

$\Rightarrow$ Probabilistic greedy algorithm

(Boyaval, Lelièvre,2010) (Cohen, Dahmen, DeVore, Nichols,2020) (Blel, Ehrlacher, Lelièvre,2021) (Cai, Yao, Liao,2022)

Probabilistic greedy algorithm (B.-F., Macherey, Nouy, Prieur,in preparation)

Start from $V_0 = \{0\}$ and proceed, for $n \geq 1$, as follows.

1) Select

$$\xi_r \in \arg\max_{\xi \in \tilde{\Xi}} \mathbb{E}(Z_{r-1}(\xi))$$

2) Compute $u(\xi_r)$ and update $V_r = \text{span}\{u(\xi_1), \ldots, u(\xi_r)\}$.

Start from $V_0 = \{0\}$ and proceed, for $n \geq 1$, as follows.

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Possible approaches.

- Crude Monte-Carlo based approach:

  ✓practically simple,
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- Bandit algorithm based approach:

  (Lattimore-Szepesvári,2022) (B.-F., Macherey, Nouy, Prieur,2022)

  ✗structural complex assumption on $Z_r(\xi)$ leading to practical limitation,
  ✓designed to return a probably approximately correct (PAC) maximum ξ_r in relative precision with adaptive number of samples.

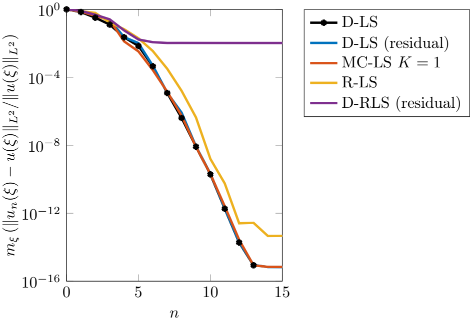
  $\Rightarrow$ Weak-greedy algorithm with high probability

Application for one-dimensional parameter-dependent advection-diffusion equation

- Snapshots are the exact solutions $u(x,\xi) = 10x\sin(x\xi), \quad \xi \in [2\pi, 4\pi]$
- Projections are computed using Least-Square (LS), Residual LS (RLS).

Confronted approaches for greedy selection.

- D: deterministic exact error
- D (residual): deterministic residual based error
- MC: FK-MC estimate with $K = 1$ sample
- R: ξ_r chosen at random in $\tilde{\Xi}$ (without replacement).



Mean relative error in L^2-norm for 100 instances of ξ, with respect to rank

1. Time independent linear problems

2. Time dependent non-linear problems

3. Conclusion

Projects: GdR MoMas (Manu) REMDYN (2015), PEPS DROME by the Cellule Energie du CNRS (2019) with T. Heuzé.

(B.-F., Nouy,2017) (B.-F., Falcò, Nouy,2021) (B.-F., Falcò, Nouy,2021b) (B.-F., Heuzé,preprint)

Let $T > 0$. We seek, for all $\xi \in \Xi$, $\mathsf{u}(\xi) : D \times [0, T] \to \mathbb{R}$ solution of

$$\begin{aligned} \partial_t \mathsf{u}(t,\xi) &= \mathcal{A}(\xi)\mathsf{u}(t,\xi) + \mathsf{h}(u(t,\xi), t, \xi), \quad \text{in } D \times (0,T], \\ \mathsf{u}(0,\xi) &= \mathsf{u}^0(\xi), \end{aligned} \tag{9}$$

with suitable boundary conditions. Here $\mathsf{h} : \mathbb{R} \times [0, T] \times \Xi \to \mathbb{R}$ and $\mathsf{u}_0 : D \times \Xi \to \mathbb{R}$.

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Local (in time), linear approximation.

At each time t, we seek $u_r(t)$ as the rank-r approximation of $u(t) \in X := V \otimes S$, i.e.

$$u_r(t, \xi) = \sum_{i=1}^{r} \alpha_i(t, \xi) v_i(t)$$

where $\{v_1(t), \ldots, v_r(t)\} \subset V$ and $\{\alpha_1(t), \ldots, \alpha_r(t)\} \subset S$.

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Dynamical low-rank approximation (DLRA) methods.

(Koch, Lubich,2007) (Nonnenmacher, Lubich,2008) (Sapsis, Lermusiaux,2009) (Cheng, Hou, Zhang, Sorensen,2013) (Musharbash, Nobile, Zhou,2015) (Feppon, Lermusiaux,2018)...

1. Approximation in low-rank tensor subset
2. Projection based method in low-dimensional subspaces

Let $X = \mathbb{R}^{n\times m}$, we seek $u : [0,T] \to X$ s.t.

$$\dot{u}(t) = f(u(t),t), t \in (0,T] \tag{10}$$

with $u(0) = u^0 \in \mathbb{R}^{n\times m}$ and $f : \mathbb{R}^{n\times m} \times [0,T] \to \mathbb{R}^{n\times m}$.

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Tensor subset. We consider the set of rank-r matrices

$$\mathcal{M}_r(\mathbb{R}^{n \times m}) = \{v \in \mathbb{R}^{n \times m} : \operatorname{rank}(v) = r\} \subset X.$$

① Dynamical low-rank approximation in tensor subsets

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Dirac-Frenckel variational principle. We seek a $u_r(t) \in \mathcal{M}_r(\mathbb{R}^{n\times m})$ as

$$\dot{u}_r(t) = \arg \min_{\dot{v} \in \mathrm{T}_{u_r(t)}\mathcal{M}_r(\mathbb{R}^{n\times m})} \|\dot{v} - f(u_r(t),t)\|_F, \; t \in (0,T], \tag{11}$$

with $\mathrm{T}_{u_r}\mathcal{M}_r(\mathbb{R}^{n\times m})$ the tangent space to $\mathcal{M}_r(\mathbb{R}^{n\times m})$ at u_r.

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Equivalently,

$$\dot{u}_r(t) = P_{\mathrm{T}_{u_r(t)}} f(u_r(t),t), \tag{12}$$

with $P_{\mathrm{T}_{u_r(t)}}$ the orthogonal projection on the tangent space.

How to solve (matrix) differential equation (12) ?

Riemaniann based time-stepping schemes.

a. Work in the ambiant space $\mathbb{R}^{n\times m}$
b. Update/projection steps for u_r with explicite Runge Kutta scheme

(Kieri, Vandereycken,2019)...

"Geometry" based approaches.

a. Suitable parametrization of $\mathcal{M}_r(\mathbb{R}^{n\times m})$
b. Suitable numerical discretization using projector splitting schemes

Parametrization of $\mathcal{M}_r(\mathbb{R}^{n\times m})$. Any $u_r \in \mathcal{M}_r(\mathbb{R}^{n\times m})$ may be decomposed as

$$u_r = \mathsf{UGV}^T,$$

with $\mathsf{U} \in \mathcal{M}_r(\mathbb{R}^{n\times r}), \mathsf{V} \in \mathcal{M}_r(\mathbb{R}^{m\times r})$ and $\mathsf{G} \in \mathrm{GL}_r$.

✗ But this decomposition is not unique!

ⓐ Suitable geometric description of $\mathcal{M}_r(\mathbb{R}^{n\times m})$

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✗ But this decomposition is not unique!

Possible paths.

1. Impose the so-called gauge conditions through tangent space (Koch,Lubich,2007)
2. Use chart based geometric description of $\mathcal{M}_r(\mathbb{R}^{n\times m})$ (B.-F., Falcò, Nouy,2021)

   $\Rightarrow$ We recover naturally gauge conditions!

Especially, $\dot{u}_r \in \mathrm{T}_{u_r}\mathcal{M}(\mathbb{R}^{n\times m})$ is uniquely given by

$$\dot{u}_r = \mathsf{U}_\perp \dot{\mathsf{X}}\mathsf{G}\mathsf{V}^T + \mathsf{U}\mathsf{G}(\mathsf{V}_\perp \dot{\mathsf{Y}})^T + \mathsf{U}\dot{\mathsf{H}}\mathsf{V}^T,$$

with $\mathsf{U}_\perp \in \mathcal{M}_{n-r}(\mathbb{R}^{n\times(n-r)}), V_\perp \in \mathcal{M}_{m-r}(\mathbb{R}^{n\times(m-r)})$, $\mathsf{U}_\perp^T\mathsf{U} = 0$ and $\mathsf{V}_\perp^T\mathsf{V} = 0$, and

$$\begin{aligned} \dot{\mathsf{X}} &= \mathsf{U}_\perp^+ f(u_r)(\mathsf{V}^+)^T\mathsf{G}^{-1}, \\ \dot{\mathsf{Y}} &= \mathsf{V}_\perp^+ f(u_r)^T(\mathsf{U}^+)^T\mathsf{G}^{-T}, \\ \dot{\mathsf{H}} &= \mathsf{U}^+ f(u_r)(\mathsf{V}^+)^T. \end{aligned} \quad (13)$$

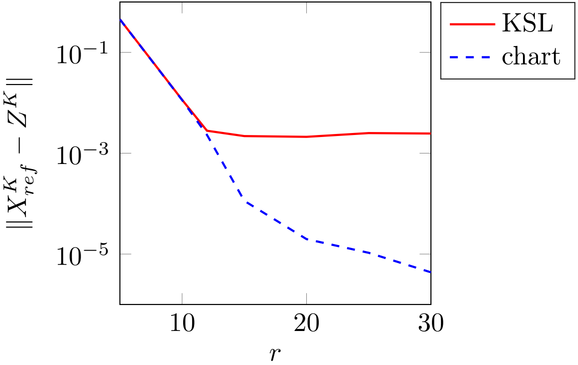
Lie-Trotter projector-splitting integrators.

- Update successively $\mathsf{X}, \mathsf{Y}, \mathsf{H}$ (or $\mathsf{U}, \mathsf{G}, \mathsf{V}$)
- Different variants depending on splitting order for $P_{\mathrm{T}_{u_r}}$

(Lubich, Oseledets,2014) (Kieri, Lubich, Walach,2014) (Ceruti, Lubich,2022) (Kazashi, Nobile, Vidličková,2021) (B.-F., Falcò, Nouy,2021b)...

Confronted approaches.

1. KSL : Symmetric splitting (Lubich, Oseledets,2014)
2. Chart: Chart based splitting algorithm



Approximation error to reference in Frobenius norm with respect to rank.

② Projection based method : time-dependent RBM (B.-F., Nouy,2017)

Let $V = \mathbb{R}^n$, for all $\xi \in \Xi$, we seek $u(\xi) : [0,T] \to V$ s.t.

$$u'(t,\xi) = f(u(t,\xi),t,\xi), \quad t \in (0,T], \tag{14}$$

with $u(0,\xi) = u_0(\xi)$ given.

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(Online) Projection step.

We are given time-dependent reduced space $V_r(t) \subset V$ with $\dim(V_r(t)) = r$.

$$\begin{cases} \alpha_i'(t,\xi) = \langle f(u_r(t,\xi),t,\xi) - \sum_{i=1}^{r} v_i'(t)\alpha_i, v_i(t)\rangle, t > 0, i = 1,\dots,r \\ \alpha_i(0,\xi) = \langle u^0(\xi), v_i(0)\rangle. \end{cases} \tag{15}$$

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(Offline) T-greedy algorithm.

Let $\tilde{\Xi} \subset \Xi$ be a discrete training set and $V_0 = \{0\}$. For $r \geq 1$ proceed as follows.

1) Select

$$\xi_r \in \arg\max_{\xi \in \tilde{\Xi}} \Delta_r^{(0,T)}(\xi).$$

2) Compute $t \mapsto u(t,\xi_r)$ and update $V_r(t) = \text{span}\{u(t,\xi_1),\dots,u(t,\xi_r)\}$.

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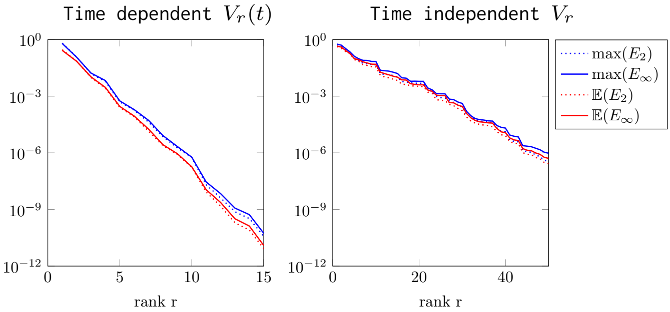
- ✓ The Galerkin projection u_r interpolates the solution u for $\{\xi_1,\dots,\xi_r\}$.
- ✓ Smaller reduced spaces for reaching the same accuracy than RBM.

One-dimensional viscous Burgers's equation with random coefficients.



Max and mean relative error for 50 instances of the parameter with respect to rank.

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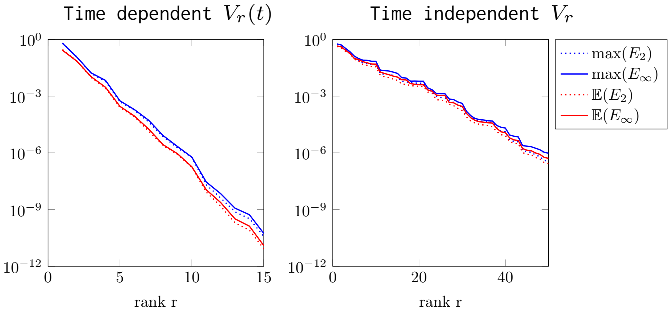

Max and mean relative error for 50 instances of the parameter with respect to rank.

Some prospects for transport. The solution manifold can not be well approximated with a single time-independent linear space V_r. (Ohlberger,Rave,2015) (Greif,Urban,2019)

- Better approximation with time-dependent reduced spaces (B.-F., Nouy,2017)
- MOR methods relying on transformed snapshots (Ohlberger, Rave,2013) (Cagniart, Crisovan, Maday, Abgrall,2017) (Rim, Peherstorfer, Mandli,2019) (Black, Schulze, Unger,2020) (Kleikamp, Ohlberger, Rave,2022)...

  $\Rightarrow$ REA method: Reconstruction approach in FV framework (B.-F., Heuzé,preprint)

Outline

1. Time independent linear problems
2. Time dependent non-linear problems
3. Conclusion

Many challenging questions for computing u_r.

- ✓ What if $y = x$ in $\Theta = D$ or $y = (x,t)$ in $\Theta = D \times I$?
- ✓ Under which form(at), do we seek the approximation u_r?
- ✓ How to compute u_r from suitable projection? optimization?
- ✓ Compute $u_r(\xi)$ from snapshots in Ξ? from pointwise evaluations over $\Theta \times \Xi$?
- ✓ Can the approximation u_r be optimal? quasi-optimal? in which sense?
- ✓ What kind of algorithms to get u_r and/or V_r? deterministic? probabilistic?
- ✓ How to deal with high dimensional problems ?

Parameter-dependent PDEs with probabilistic interpretation.

- Validate the approach in fully sample setting (ongoing work).
- Extension and validation for high dimensional cases or time-dependent problems.

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Dynamical low-rank approximation methods for parameter and time-dependent PDEs.

- Further analysis of chart based splitting approach for matrix ODEs.
- Improve computational cost of projection based methods using randomized linear algebra.
- Toward "nonlinear" approximation: applicability of REA for conservation laws, Neural Network Galerkin approach.

...

Thanks for your attention !

Publications during PhD and Post-Doctorate

M. B.-F., Stabilized finite element method for incompressible-compressible two-phase flows, PhD thesis, Université Sciences et Technologies - Bordeaux I, 2009.

M. B.-F., G. Gallice and B. Nkonga, Stabilized Finite Element Method for Compressible- Incompressible Diphasic Flows. In: Kreiss G., Lötstedt P., Målqvist A., Neytcheva M. (eds) Numerical Mathematics and Advanced Applications 2009, 2010.

M. B.-F., G. Gallice and B. Nkonga, A simple stabilized finite element method for solving two phase compressible-incompressible interface flows. Comput. Methods Appl. Mech. Eng., 2011.

M. Billaud-Friess, B. Boutin, F. Caetano, G. Faccanoni, S. Kokh, F. Lagoutière and L. Navoret, A second order anti-diffusive Lagrange-remap scheme for two-component flows. ESAIM Proc., 2011.

M. Billaud-Friess, and S. Kokh, An anti-diffusive Lagrange-Remap scheme for multi- material compressible flows with an arbitrary number of components. ESAIM Proc., 2012.

M. Billaud-Friess, J. Breil, P.-H. Maire and M. Shashkov, A Multi-Material CCALE- MOF Approach in Cylindrical Geometry. Comm. Comput. Phys., 2014.

M. Billaud-Friess, and S. Kokh, Simulation of sharp interface multi-material flows involving an arbitrary number of components through an extended five-equation model. J. Comput. Phys., 2014.

Publications since at Centrale Nantes

M. Billaud-Friess, A. Nouy and O. Zahm, Méthode de réduction de modèle a priori basée sur des formulations idéales en minimum de résidu. Actes CSMA 2013, 2013.

M. Billaud-Friess, A. Nouy, and O. Zahm, A tensor approximation method based on ideal minimal residual formulations for the solution of high-dimensional problems. ESAIM: Mathematical Modelling and Numerical Analysis - Modélisation Mathématique et Analyse Numérique, 2014.

Zahm, O., M. Billaud-Friess, and A. Nouy, Projection-Based Model Order Reduction Methods for the Estimation of Vector-Valued Variables of Interest. SIAM J. Sci. Comput., 2017.

M. Billaud-Friess, and A. Nouy, Dynamical Model Reduction Method for Solving Parameter-Dependent Dynamical Systems. SIAM J. Sci. Comput., 2017.

M. Billaud-Friess, A. Macherey, A. Nouy and C. Prieur, Stochastic Methods for Solving High-Dimensional Partial Differential Equations. Monte Carlo and Quasi-Monte Carlo Methods. MCQMC 2018, 2020.

M. Billaud-Friess, A. Falcó, and A. Nouy, Principal bundle structure of matrix manifolds. MDPI, Mathematics, 2021.

M. Billaud-Friess, A. Falcó, and A. Nouy, A new splitting algorithm for dynamical low-rank approximation motivated by the fibre bundle structure of matrix manifolds. Bit Numer. Math., 2021.

M. Billaud-Friess, A. Macherey, A. Nouy and C. Prieur, A PAC algorithm in relative precision for bandit problem with costly sampling., Mathematical Methods of Operations Research, 2022.

M. Billaud-Friess, and T. Heuzé, Reconstruction of finite volume solution for parameter-dependent linear hyperbolic conservation laws. arXiv, 2006.1035 (preprint)

M. Billaud-Friess, A. Macherey, A. Nouy and C. Prieur, A probabilistic reduced basis method for parameter-dependent problems. (in preparation)