What Markus did, does and shall do

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Benasque, 03.09.2009

I work on an IPOD

that so far

does not play music.

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Motivation of POD in Context of PDE

1. **(Vertical) Method of Numerical Treatment of PDE:**
   - Galerkin Ansatz with finite dimensional test space (say FE)
   - Choice of basis functions $\rightsquigarrow$ System of ODEs
   - Solve ODEs for coefficients of that basis (many in FE case!)
2. **Idea of POD Reduced-order Modeling:**
   - Determine "intelligent" basis which contains characteristics of the expected solution
   - Obtain a low dimensional problem in the respective coefficients
   - Hope: #POD-Basis $\ll$ #FE-Basis
3. **Method:**
   - Take "snapshots" of the PDE (FE-)solution y
   - POD: Extract key ingredients to determine an "optimal" basis
   - Use the span of this basis as test space in Galerkin (Project the dynamical system on the span)

Problem for optimization:
Snapshots may not be valid for all choices of controls

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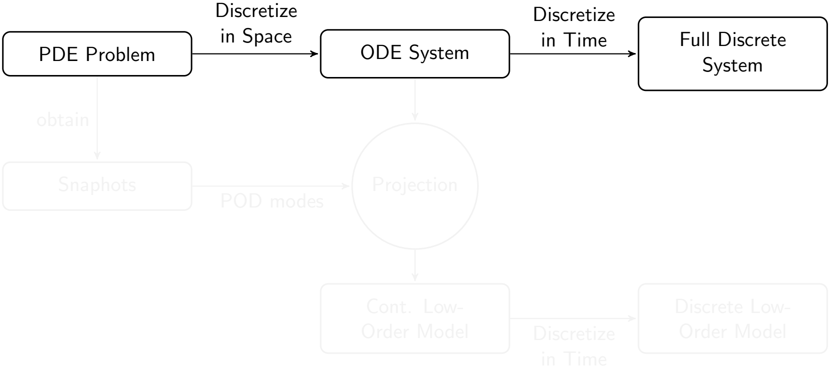
Overview of POD Reduced-Order Modeling



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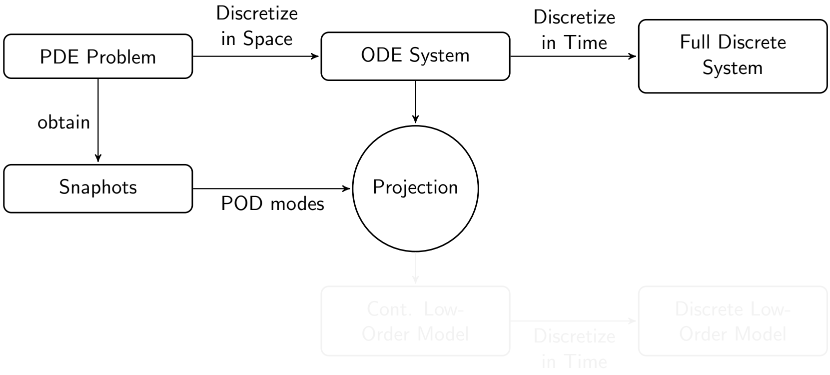

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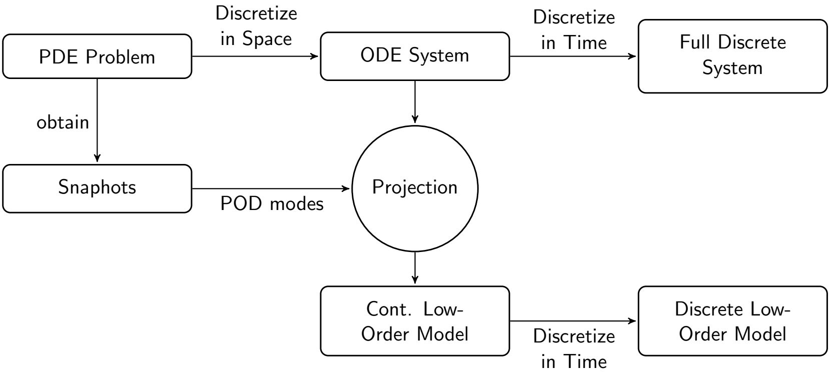

POD for FE Discretizations

- **Snapshot Locations:** $\{t_j\}_{j=1}^n \subset [0, T]$
- **Snapshot Ensemble:** $\mathcal{V} :=$ span$\{y_j : y_j$ FE vector at $t_j\}_{j=1}^n$
- **Projection:** $P^\ell y = \sum_{k=1}^{\ell} (y, \psi_k)_X \, \psi_k$ for $X = V_h$ or $X = H_h$
- **Aim:** On average, best approximate $\mathcal{V}$ by $\mathcal{V}^\ell :=$ span(B^ℓ), with ONB $B^\ell = \{\psi_k\}_{k=1}^{\ell}$
- **POD Problem:**

$$\min_{B^\ell} \sum_{j=1}^{n} \alpha_j \left\| y_j - P^\ell y_j \right\|_X^2 \quad \text{s. t.} \quad (\psi_i, \psi_j)_X = \delta_{ij}$$

- **Solution:**
  - $\{\psi_k\}_{k=1}^{\ell}$ is given by the "largest" ℓ left singular vectors of essentially the Ensemble matrix $Y := [y_1, \ldots, y_n]$
  - These vectors may be characterized by the EVP

$$R_h = YY^T \psi_i = \lambda_i \psi_i, \qquad i = 1, \cdots, \ell$$

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Optimal Control Problem

1. **Linear-Quadratic Control Problem:**
   For $\mathcal{U}_{ad} \subset \mathcal{U}$ closed, *convex*, nonempty:

$$\min_{u \in \mathcal{U}_{ad}} J(y,u) = \frac{\beta}{2} \int_0^T \|y(t) - z(t)\|_H^2 \, dt + \frac{1}{2} \|u\|_{\mathcal{U}}^2$$

   s. t $(y,u) \in W(0,T) \times \mathcal{U}_{ad}$ solves

$$\begin{aligned} \frac{d}{dt}(y(t),\varphi)_H + a(y(t),\varphi) &= \langle u(t),\varphi \rangle_{V',V}, \quad && \varphi \in V, t \in [0,T] \\ (y(0),\varphi)_H &= (y_0,\varphi)_H, && \varphi \in V \end{aligned}$$

2. **Suboptimal Control:**
   Choose $V := \mathcal{V}^\ell = \text{span}(\{\psi_k\}_{k=1}^\ell)$
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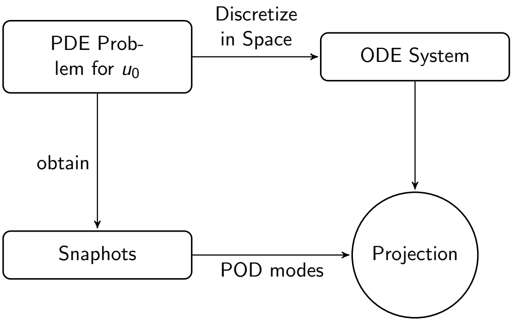
Adaptive POD Algorithm – Problem with Basis Update



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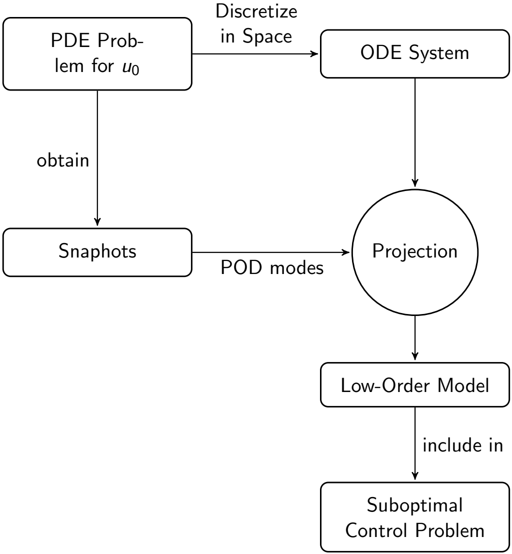

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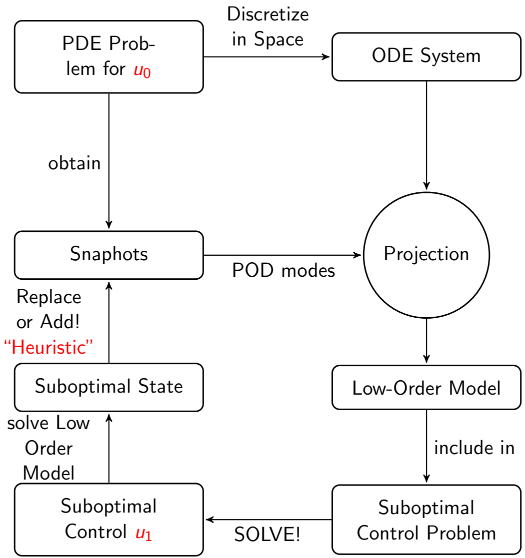

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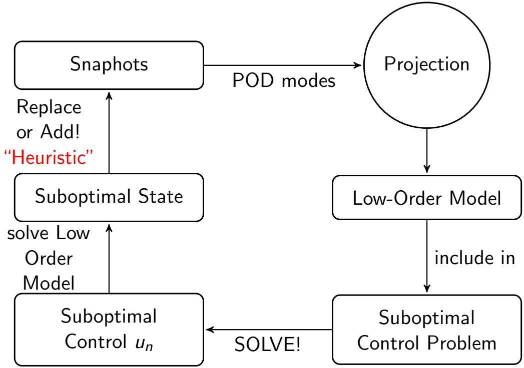

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OS-POD Statement

For (y^ℓ, u) and (y, ψ^i, λ^i), $\min J(y^\ell, u)$ subject to

- **POD ROM** (for $t \in (0, T]$ plus IC^ℓ)

$$\frac{\partial}{\partial t} y^\ell(t) = P^\ell_{y(u)}\big(F(y^\ell(t)) + Bu(t)\big)$$

- **Full State** (for $t \in (0, T]$ plus IC)

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- **POD Basis Condition**

$$R_{y(u)}\psi^i = \lambda^i \psi^i \qquad \text{for } i = 1, \ldots, \ell$$

$$\left(\psi^i, \psi^j\right)_X = \delta_{ij} \qquad \text{for } i, j = 1, \ldots, \ell$$

- **Defining**

$$Rv := \int_0^T (v, y(u))_X\, y(u)\, dt, \quad P^\ell_{y(u)} w := \sum_{k=1}^{\ell} \left(\psi^\ell_{y(u)}, w\right)_X \psi^\ell_{y(u)}$$

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Remarks on OS-POD

- **Established Analysis**
  - For fixed ℓ, convergence is shown by Kunisch/Volkwein '08
  - For fixed u, convergence is shown for $\ell \to \infty$ (Henri '03)
- **TODO**
  - Convergence of OS-POD w.r.t. $\ell \to \infty$
  - Analysis for "non-continuous" POD (not "all snapshots")
  - Including a POD System for the adjoint state?!
- **Discussion**
  - Basis is updated without "engineering"
  - Problem size is significantly increased:
    Eigenvalue Problem and full system solve included
- **Numerical Results**

  Kunisch/Volkwein '08:

  "Control of non-stationary burger's equation"

  Speedup factor in comparison to FE-SQP: 2 and 6

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- **Idea:**
  Apply OSPOD to equation which challenges POD-ROM
- **Problem:**
  Extremly simplyfied "Monodomain Equation"
  (Essentially HEq with strong non-linearity)
- **Challenge:**
  - POD Basis represents time-averaged spatially shifted correlation of snapshot data
  - Correlation for snapshots very small
    $\rightsquigarrow$ POD does not perform well
- **Numerical Result:**
  - Also in interaction with D. Chapelle, INRIA France
  - 1D-FE solution, RK or θ-scheme
  - Rather poor approximation for large basis: $\ell = 26$
    $\rightsquigarrow$ computation time even lengthened(!)
  - Possibly "direction" not modeled correctly

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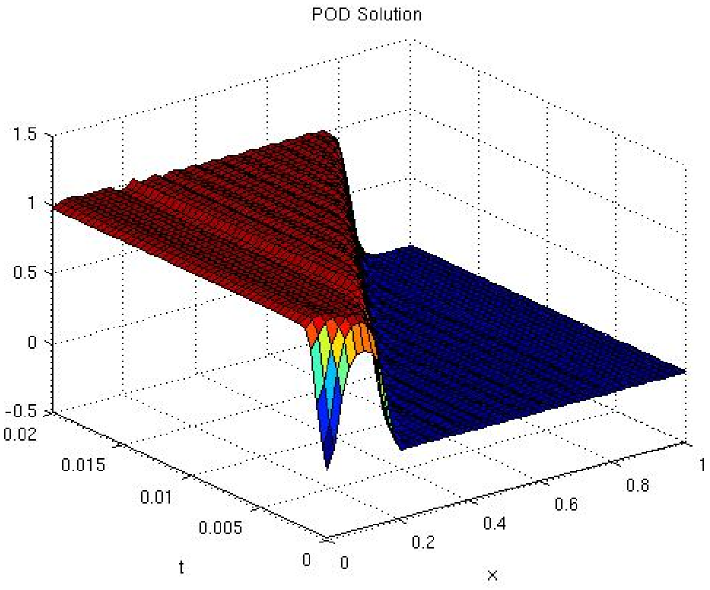
POD Approximation of FHN Solution ($\ell = 26$)



What to Take Home

- **POD Method**
  - "POD" essentially means "SVD"
  - "POD-ROM":
    Collect n snapshots of a dynamical system in ensemble matrix.
    Use ℓ "largest" singular vectors as a Galerkin basis for ROM.
  - Representation of snapshots(!) is optimal for its rank
- **POD Suboptimal Control**
  - Main problem: Basis Update
    $\rightsquigarrow$ Possible way out: OS-POD
  - Basis updated such that at the optimal solution, the basis represents the key dynamics of the optimal state
  - Drawback: Computational effort increased
- **Open Problems?**
  - Convergence analysis of OS-POOD for $\ell \to \infty$
  - OS-POD performance for challenging FHN model

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- **Compartment model**
  - Together with Prof Keeling and Henry Kasumba, Graz
  - Establish exponential decay for solution of a convection-diffusion system in semi-group framework
- **Closed-Loop Control**
  - Involves Hamilton Jacobi Bellman Equation
  - Typical feasible dimensions of system are 5 to 10 $\rightsquigarrow$ Model reduction highly desired
  - POD studied in this context by Kunisch/Xie '04
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  - Providing "Student's Union for Research"
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Presentation and Layout of Mathematical Writing

- Understanding mathematical structures with less effort
  $\rightsquigarrow$ Roles of items? Ideas? "Simply" conclusions?
  $\rightsquigarrow$ Interaction of text and diagrams (LaTeX-Extensions)
- Let students design/refine diagrams
  $\rightsquigarrow$ Interpretation skills improved
  $\rightsquigarrow$ Improve literature by studying it
- Let (non-expert) recipient be aware of whole situation
  $\rightsquigarrow$ Decide what to understand – Organizing what to tell
  $\rightsquigarrow$ Pyramid structure
- Finally, create global "Mathematical Knowledge Base"
  - Represent diagrams in multi-user DAG/database
  - Understand Lemma/Proposition/Proof as "Clustering"
  - "Classical documents" are reports from database

  $\rightsquigarrow$ Interactively zoomable Googlemaps of MathWorld

First "Layout-Draft" in Diploma Thesis

Further Interpretation of the POD – Autocorrelation Let us now draw a connection of the POD to autocorrelation by "interpreting" the POD operator. In particular, we introduce a kernel r which is of the form of an autocorrelation (defined in (A.1)).

Corollary A.1.2 (Autocorrelation Property)
The POD operator R_L is an integral operator whose kernel may be represented by an *averaged autocorrelation* function $r : \Omega \times \Omega \to \mathbb{R}$ (w.r.t. the snapshots). In particular, for $\psi \in L^2(\Omega)$, the operator R_L may be written as

$$(R_L\psi)(x) = \int_\Omega \psi(z)\, r(x,z)\, \mathrm{d}z \quad \text{with} \quad r(x,z) := \langle\, y(t)(x)\, y(t)(z)\, \rangle_{t\in\Gamma}\,. \tag{A.2}$$

Proof.
Recall that in the definition of a POD Problem, the average operation was assumed to commute with the inner product. We may thus obtain the assertion by swapping the average operation and the integration in the definition of the operator R_L in Corollary A.1.1. □

Decomposition of Autocorrelation We have seen that the kernel of the POD operator is given by an autocorrelation operator. We now wish to show that the POD modes actually decompose this autocorrelation operator. (This result will enable us to prove that Coherent Structures (in the sense proposed by Sirovich) may be obtained by POD modes.)
We prove this result in the fashion proposed in Volkwein 1999. Note however that the assertion may also be obtained by means of "functional analysis" – in particular, the so called *Mercer's Theorem*.

Proposition A.1.3 (Decomposition of the Autocorrelation Operator)
Let $\mathcal{B}^\ell = \{\psi_k\}_{k=1}^{\ell}$ denote a POD Basis determined by R_L. Let r be the kernel of R_L in the sense of Corollary A.1.2. Then, there holds

$$r(x,z) = \sum_{k\in\mathbb{N}} \lambda_k \psi_k(x)\psi_k(z). \tag{A.3}$$

Mathematical truth is not a matter of taste.

Its presentation is.

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Many thanks for your attention!