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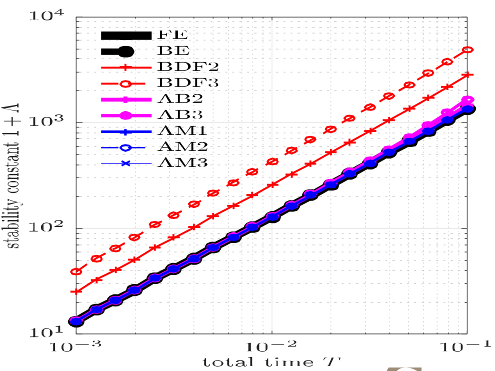
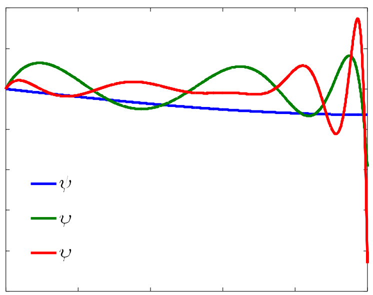
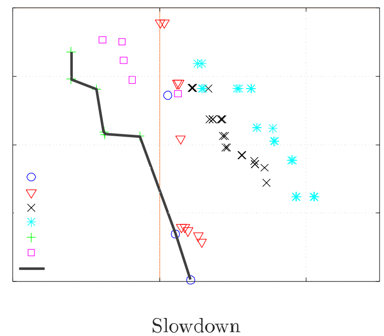
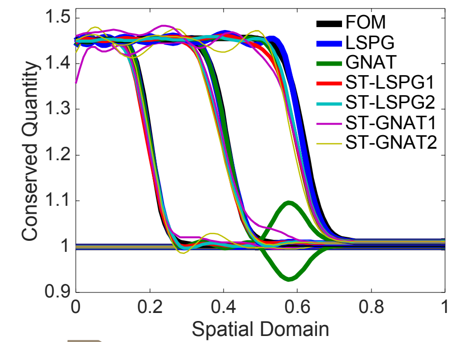




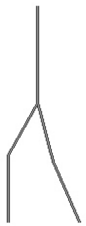


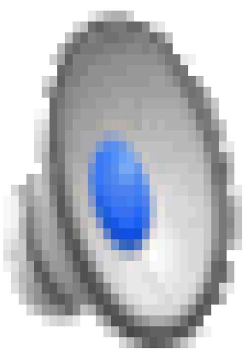


Space-time least-squares Petrov-Galerkin nonlinear model reduction

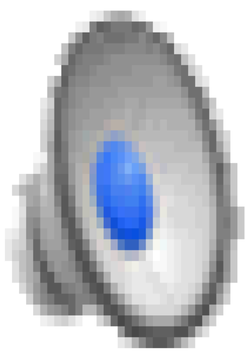
Youngsoo Choi and Kevin Carlberg

Nonlinear dynamical systems





Courtesy: K. Carlberg

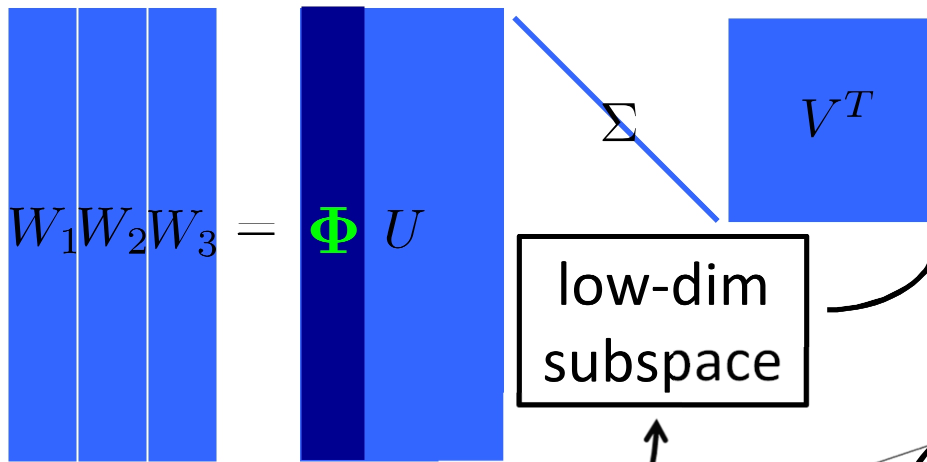


Courtesy: K. Carlberg

Reduced Order Model (ROM)

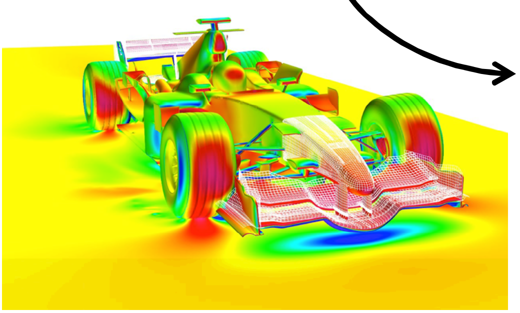
Goal: exploit data to drastically reduce simulation costs and achieve a good accuracy

high fidelity models / experiments



low-dim subspace

project & propagate in time

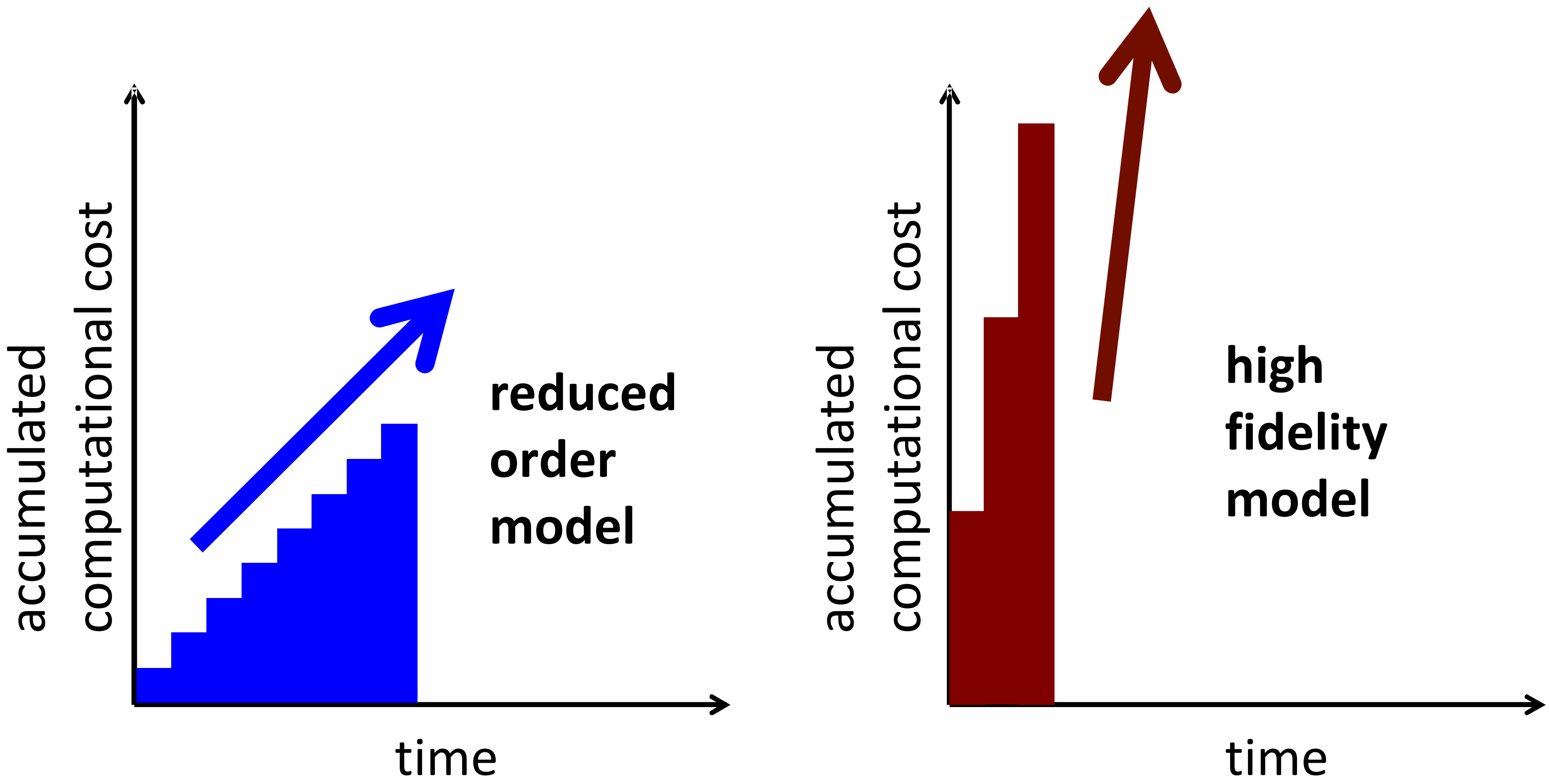


Courtesy: C. Farhat

collect & compress data

dynamical system solution

Complexity in time



Captive-carry simulation

Pressure field | Vorticity field

GNAT ROM

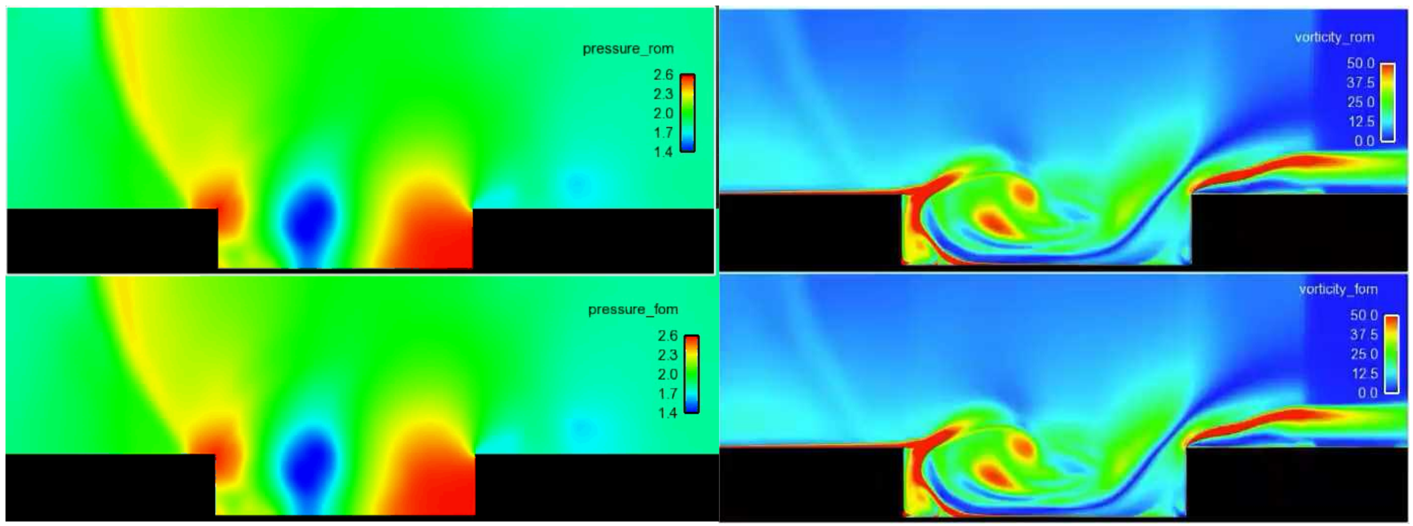
32 min, 2 cores

Courtesy: K. Carlberg

High-fidelity

5 hours, 48 cores

Courtesy: M. Barone



+ 229x savings in core–hours

Motivation for space–time ROM

- Typical ROMs apply spatial projection
  - \+ Reduces spatial computational complexity
  - \- Does not reduce temporal complexity (number of time steps remains large)
- Larger time steps with explicit time integration [Krysl et al., 2001]
  - \+ Larger stable time steps achievable with ROMs
  - \- Speedup limited by stability
  - \- Not applicable to stiff dynamics
- Space–time reduced-basis [Urban/Patera 2012], [Yano 2014], [Yano/Patera/Urban 2014]
  - \+ Dimensionality reduction in both space and time
  - \+ Error bounds grow linearly in time
  - \- *Not always practical*: requires space–time discretization in full-order model
- Forecasting with time–domain data [Carlberg/Ray/van Bloemen Waanders 2015], [Carlberg/Brencher/Haasdonk/Barth 2016]
  - \+ *Practical:* does not require space–time discretization in full-order model
  - \- *Limited reduction*: no temporal projection pursued

Goal for space–time ROM

+ Reduction both on space and time
+ Complexity is independent of both space and time
+ Amenable to any time integrator
+ Does not require a space–time full-order model
+ Slow time growth in error bound

A system of nonlinear ODEs

$$\frac{d\boldsymbol{w}}{dt} = \boldsymbol{f}(\boldsymbol{w}, t; \boldsymbol{\mu})$$
$$\boldsymbol{w}(0; \boldsymbol{\mu}) = \boldsymbol{w}_0(\boldsymbol{\mu})$$

- Parameter vector, $\boldsymbol{\mu} \in \mathbb{R}^{N_p}$
- State, $\boldsymbol{w} : [0, T] \times \mathbb{R}^{N_p} \to \mathbb{R}^{N_s}$
- Initial condition, $\boldsymbol{w}_0 : \mathbb{R}^{N_p} \to \mathbb{R}^{N_s}$
- Nonlinear function, $\mathbf{f} : \mathbb{R}^{N_s} \times [0, T] \times \mathbb{R}^{N_p} \to \mathbb{R}^{N_s}$

Linear multistep schemes

$$\boldsymbol{r}^n(\boldsymbol{w}^n) := \sum_{j=0}^{k} \alpha_j \boldsymbol{w}^{n-j} - \Delta t \sum_{j=0}^{k} \beta_j \boldsymbol{f}(\boldsymbol{w}^{n-j}, t^{n-j}, \boldsymbol{\mu})$$

- Total time steps: $N_t := T/\Delta t \in \mathbb{N}$

Truncated Higher Order SVD (T-HOSVD)

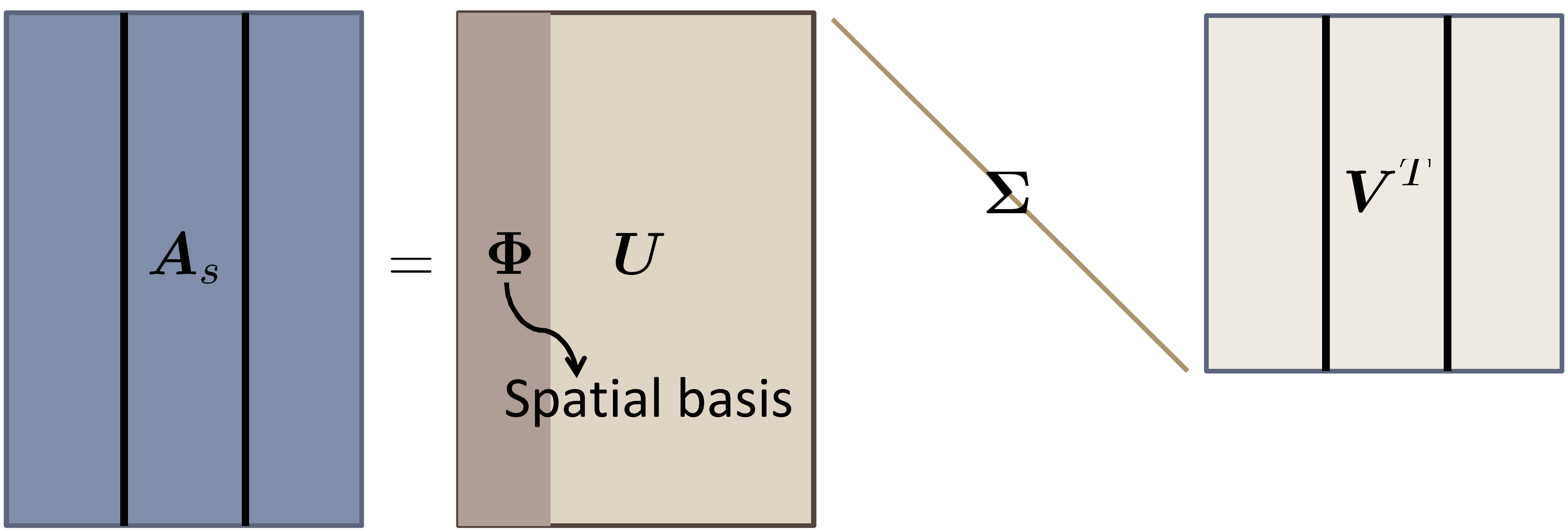
Snapshot matrix, $\boldsymbol{A}_s$

$$\boldsymbol{A}_s = \begin{bmatrix} \boldsymbol{W}_1 & \boldsymbol{W}_2 & \boldsymbol{W}_3 \end{bmatrix} - \boldsymbol{W}_{ref}$$

- Solution, $\boldsymbol{W}_i := \begin{bmatrix} \boldsymbol{w}^1(\boldsymbol{\mu}_i) & \cdots & \boldsymbol{w}^{N_t}(\boldsymbol{\mu}_i) \end{bmatrix}, \quad i \in \{1, 2, 3\}$

Singular value decomposition

$$\boldsymbol{A}_s = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$$



Fixed temporal basis, T-HOSVD

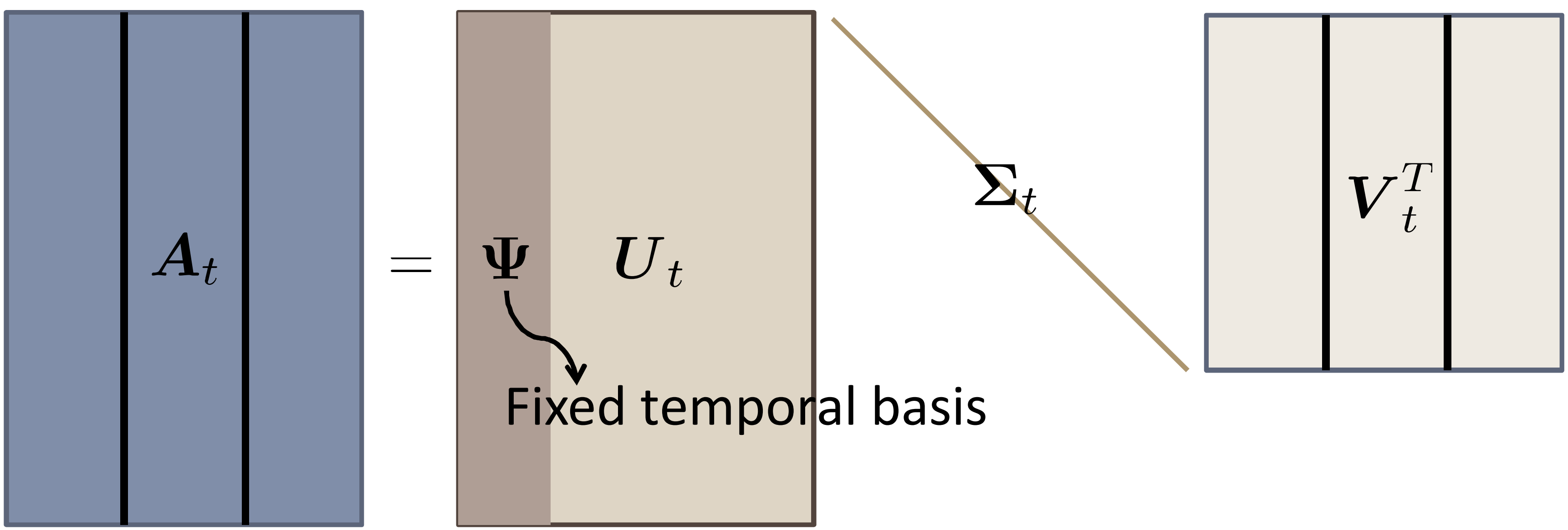
Snapshot matrix, $\boldsymbol{A}_t$

$$\boldsymbol{A}_t = \begin{bmatrix} \boldsymbol{W}_1^T & \boldsymbol{W}_2^T & \boldsymbol{W}_3^T \end{bmatrix} - \boldsymbol{W}_{ref}^T$$

- Solution, $\boldsymbol{W}_i := \begin{bmatrix} \boldsymbol{w}^1(\boldsymbol{\mu}_i) & \cdots & \boldsymbol{w}^{N_t}(\boldsymbol{\mu}_i) \end{bmatrix}, \quad i \in \{1, 2, 3\}$

Singular value decomposition

$$\boldsymbol{A}_t = \boldsymbol{U}_t \boldsymbol{\Sigma}_t \boldsymbol{V}_t^T$$



Sequentially Truncated HOSVD (ST-HOSVD)

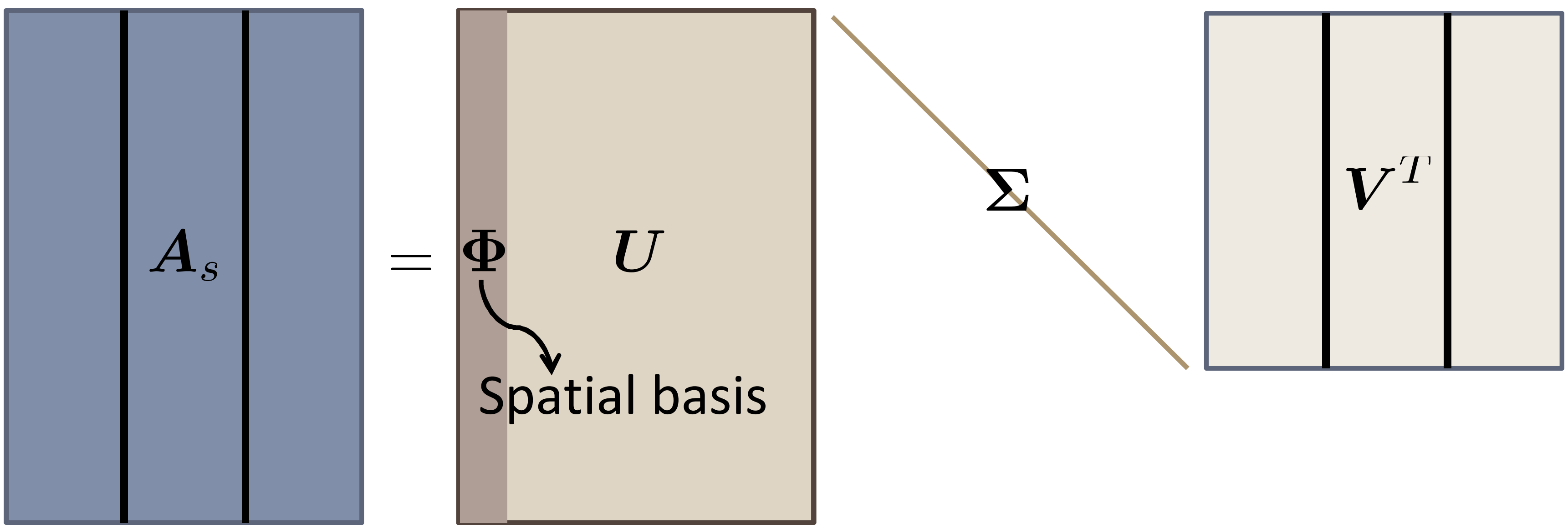
Snapshot matrix, $\boldsymbol{A}_s$

$$\boldsymbol{A}_s = \begin{bmatrix} \boldsymbol{W}_1 & \boldsymbol{W}_2 & \boldsymbol{W}_3 \end{bmatrix} - \boldsymbol{W}_{ref}$$

- Solution, $\boldsymbol{W}_i := \begin{bmatrix} \boldsymbol{w}^1(\boldsymbol{\mu}_i) & \cdots & \boldsymbol{w}^{N_t}(\boldsymbol{\mu}_i) \end{bmatrix}, \quad i \in \{1, 2, 3\}$

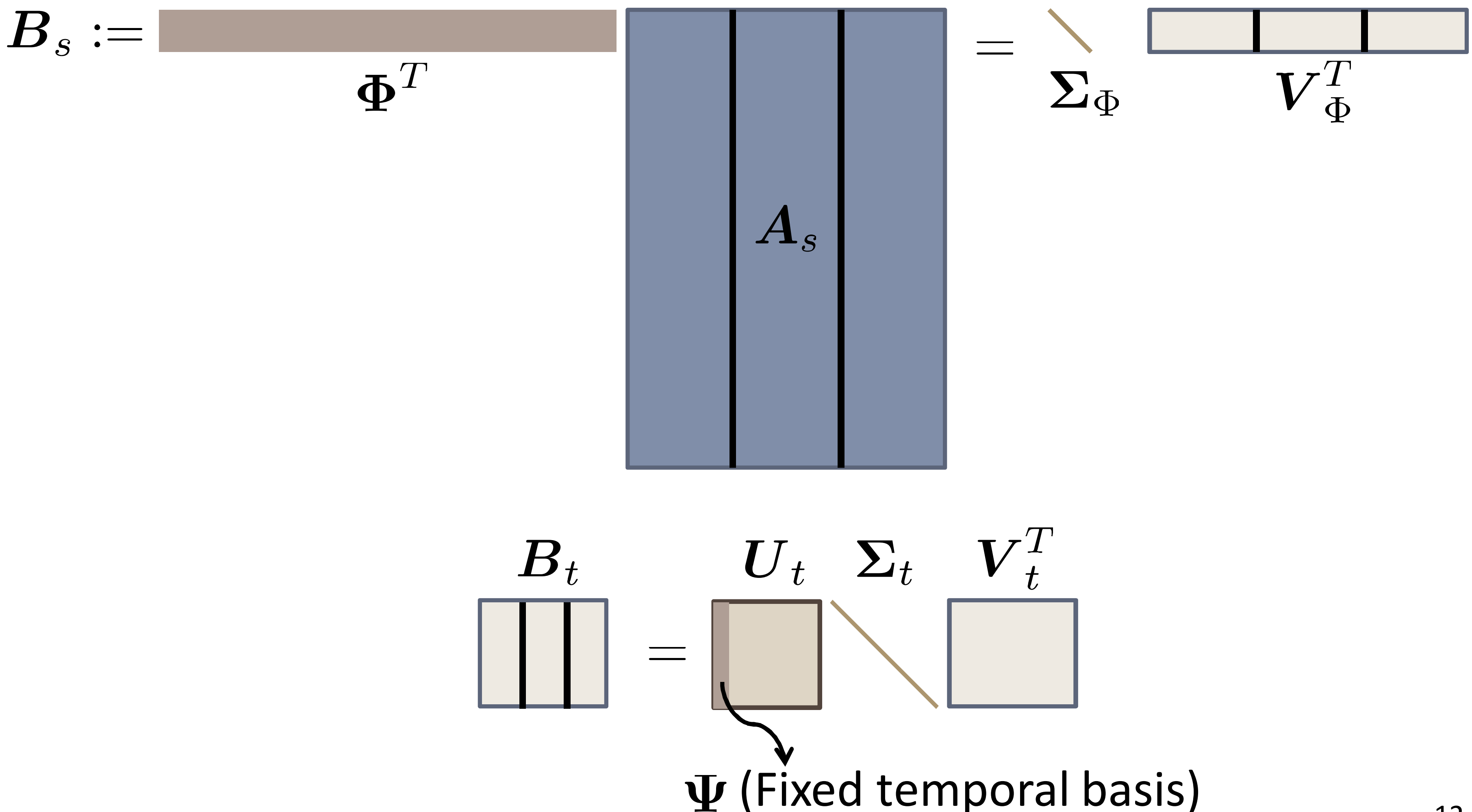
Singular value decomposition

$$\boldsymbol{A}_s = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$$



Sequentially Truncated HOSVD (ST-HOSVD)

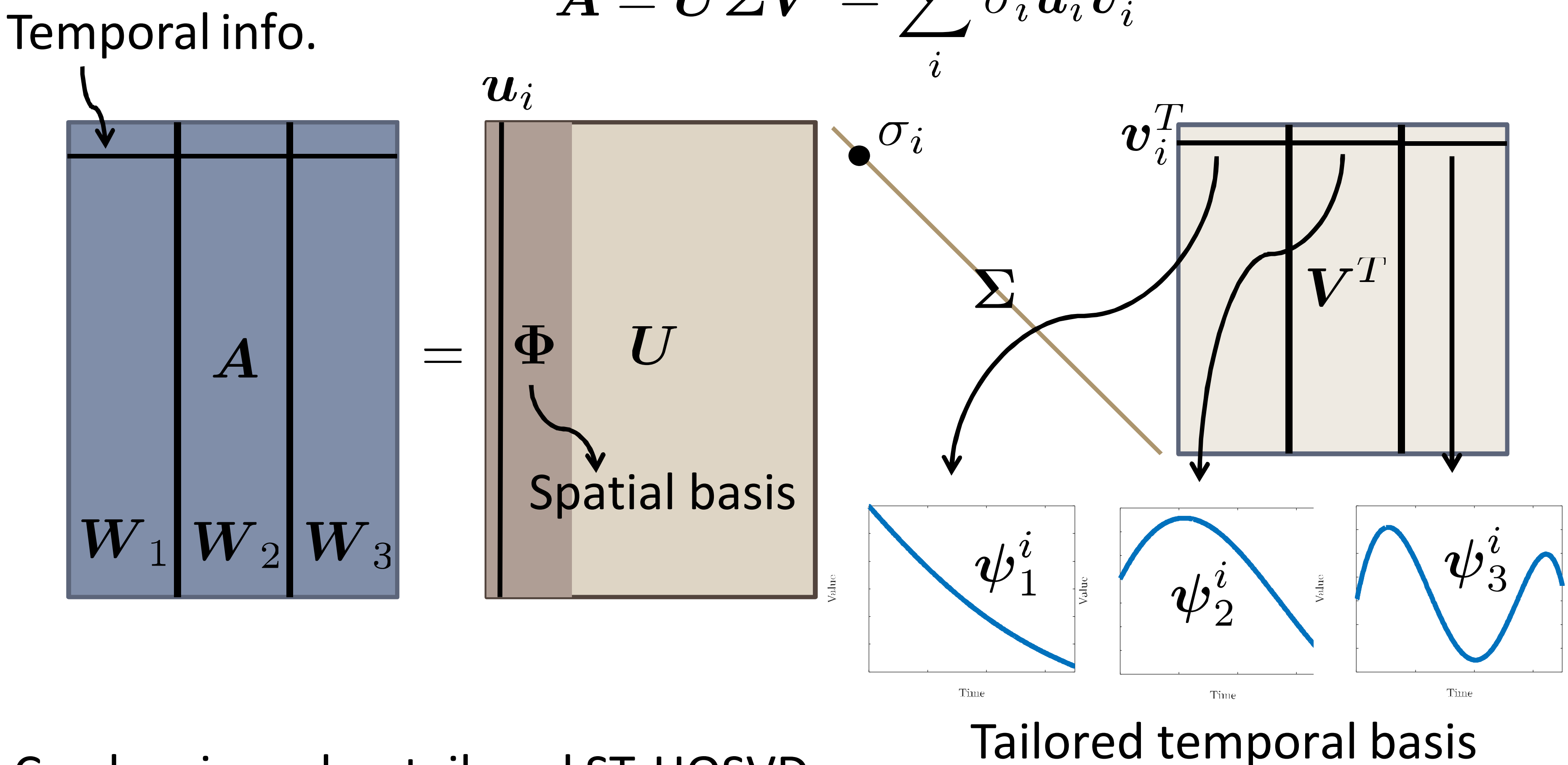
$$\boldsymbol{B}_s := \boldsymbol{\Phi}^T \boldsymbol{A}_s = \boldsymbol{\Sigma}_\Phi \boldsymbol{V}_\Phi^T$$



Tailored temporal basis

Singular value decomposition

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T = \sum_i \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T$$



Can be viewed as tailored ST-HOSVD

Tailored spatiotemporal basis

- Tailored basis, $\boldsymbol{\Upsilon}_{tailored}$

$$\begin{bmatrix} \boldsymbol{\psi}_1^1 \otimes \boldsymbol{\phi}_1 & \cdots & \boldsymbol{\psi}_{n_t^1}^1 \otimes \boldsymbol{\phi}_1 & \cdots & \boldsymbol{\psi}_1^{n_s} \otimes \boldsymbol{\phi}_{n_s} & \cdots & \boldsymbol{\psi}_{n_t^{n_s}}^{n_s} \otimes \boldsymbol{\phi}_{n_s} \end{bmatrix}$$

\+ Provides a tailored temporal basis for each spatial basis
\+ No extra expensive SVD is required
\- The dimension of temporal basis $\leq n_\mu$

Fixed spatiotemporal basis

- Fixed basis, $\boldsymbol{\Upsilon}_{fixed}$

$$\left[\boldsymbol{\psi}_1 \otimes \boldsymbol{\phi}_1 \quad \cdots \quad \boldsymbol{\psi}_{n_t} \otimes \boldsymbol{\phi}_1 \quad \cdots \quad \boldsymbol{\psi}_1 \otimes \boldsymbol{\phi}_{n_s} \quad \cdots \quad \boldsymbol{\psi}_{n_t} \otimes \boldsymbol{\phi}_{n_s}\right]$$

+ The dimension of temporal basis $< N_s n_\mu$
- Requires an extra expensive SVD
- No tailored temporal basis available

Trial subspace

Spatial ROM

- Solution approximation:

$$\tilde{\boldsymbol{w}} \in \underbrace{\boldsymbol{w}_{ref} \otimes \mathbf{1}_{N_t} + \mathcal{S} \otimes \mathbb{R}^{N_t}}_{\text{space–time subspace}} \subseteq \underbrace{\mathbb{R}^{N_s} \otimes \mathbb{R}^{N_t}}_{\text{FOM subspace}}$$

$$\Updownarrow$$

$$\tilde{\boldsymbol{w}}(t^n) = \boldsymbol{w}_{ref} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}(t^n)$$

- Spatial subspace

$$\mathcal{S} = \mathrm{Ran}(\boldsymbol{\Phi}) \subseteq \mathbb{R}^{N_s}, \ \dim(\mathcal{S}) = n_s$$

- # degrees of freedom

$$\dim(\mathcal{S} \otimes \mathbb{R}^{N_t}) = n_s N_t$$

\- Ignores temporal reduction

Spatiotemporal ROM

- Solution approximation:

$$\tilde{\boldsymbol{w}} \in \underbrace{\boldsymbol{w}_{ref} \otimes \mathbf{1}_{N_t} + \oplus_{i=1}^{n_s} \mathcal{S}_i \otimes \mathcal{T}_i}_{\text{space–time subspace}} \subseteq \underbrace{\mathbb{R}^{N_s} \otimes \mathbb{R}^{N_t}}_{\text{FOM subspace}}$$

$$\Updownarrow$$

$$\tilde{\boldsymbol{w}} = \boldsymbol{w}_{ref} \otimes \mathbf{1}_{N_t} + \sum_{i=1}^{n_s} \sum_{j=1}^{n_t^i} \left(\boldsymbol{\psi}_j^i \otimes \boldsymbol{\phi}_i\right) \hat{w}_{ij}$$

- Spatial subspace

$$\mathcal{S}_i := \mathrm{span}(\boldsymbol{\phi}_i) \subset \mathbb{R}^{N_s}, i = 1, \ldots, n_s, \dim \mathcal{S}_i = 1$$

- Temporal subspace

$$\mathcal{T}_i := \mathrm{Ran}\left(\begin{bmatrix} \boldsymbol{\psi}_1^i & \cdots & \boldsymbol{\psi}_{n_t^i}^i \end{bmatrix}\right) \subset \mathbb{R}^{N_t}, i = 1, \ldots, n_s$$

- # degrees of freedom

$$\dim(\oplus_{i=1}^{n_s} \mathcal{S}_i \otimes \mathcal{T}_i) = \sum_{i=1}^{n_s} n_t^i$$

\+ Fewer degrees of freedom

LSPG projection

Spatial LSPG

- discrete-residual minimization

$$\hat{\boldsymbol{w}}^n = \arg\min_{\boldsymbol{y}} \|\boldsymbol{G}\boldsymbol{r}^n(\boldsymbol{w}_{ref} + \boldsymbol{\Phi}\boldsymbol{y})\|_2^2$$

- LSPG: $\boldsymbol{G} = \boldsymbol{I} \in \mathbb{R}^{N_s \times N_s}$
- Collocation: $\boldsymbol{G} = \boldsymbol{Z} \in \mathbb{R}^{n_z \times N_s}$
- GNAT: $\boldsymbol{G} = (\boldsymbol{Z}\boldsymbol{\Phi}_r)^\dagger \boldsymbol{Z}$

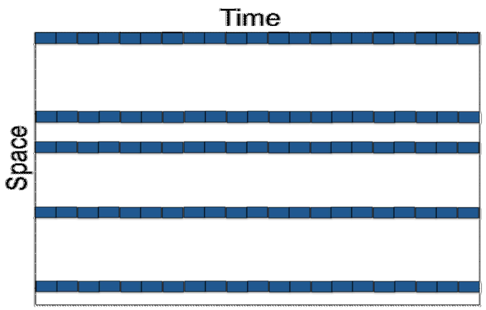


Figure: Spatial GNAT Z

\- No temporal complexity reduction

Spatiotemporal LSPG

- discrete-residual minimization

$$\hat{\boldsymbol{w}}_{\text{st}} = \arg\min_{\hat{\boldsymbol{y}}} \left\| \bar{\boldsymbol{G}}\bar{\boldsymbol{r}} \left(\boldsymbol{w}_{ref} \otimes \boldsymbol{1}_{N_t} + \sum_{i=1}^{n_s} \sum_{j=1}^{n_t^i} (\boldsymbol{\psi}_j^i \otimes \boldsymbol{\phi}_i) \hat{y}_{ij} \right) \right\|_2^2$$

- LSPG: $\bar{\boldsymbol{G}} = \boldsymbol{I} \in \mathbb{R}^{N_s N_t \times N_s N_t}$
- Collocation: $\bar{\boldsymbol{G}} = \bar{\boldsymbol{Z}} \in \mathbb{R}^{n_{\bar{z}} \times N_s N_t}$
- GNAT: $\bar{\boldsymbol{G}} = (\overline{\boldsymbol{Z}\boldsymbol{\Phi}}_r)^\dagger \bar{\boldsymbol{Z}}$

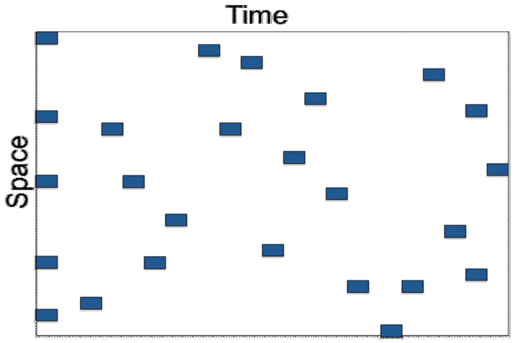


Figure: Spatiotemporal GNAT $\bar{Z}$

\+ More complexity reduction

Error bound, linear multistep

Spatial LSPG [Carlberg et al., 2016]

$$\|\boldsymbol{w}_\star^n - \tilde{\boldsymbol{w}}_{PG}^n\|_2 \leq \sum_{j=0}^{n-1} \sum_{\ell=0}^{\min(k,j)} \epsilon_\ell^{n-j+\ell} \|(\boldsymbol{I} - \mathbb{P}^{n-j+\ell})\boldsymbol{f}(\tilde{\boldsymbol{w}}_{PG}^{n-j})\|_2$$

- Exponential growth in time

Spatiotemporal LSPG

$$\|\bar{\boldsymbol{w}}_\star - \bar{\boldsymbol{w}}_{PG}\|_2 \leq \frac{\Delta t}{h} \|(\boldsymbol{T}_{LM}^{-1}\boldsymbol{F}_{LM} - \mathbb{P})\bar{\boldsymbol{f}}(\bar{\boldsymbol{w}}_{PG})\|_2$$

+ Slower stability-constant growth in time

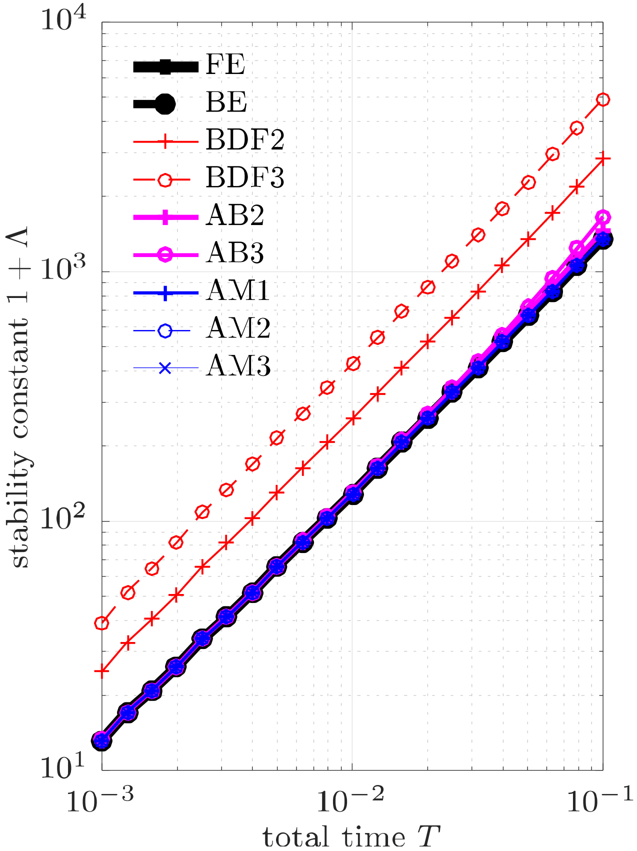
- A priori error bound with respect to ℓ_2-optimal solution

$$\|\bar{\boldsymbol{w}}_\star - \bar{\boldsymbol{w}}_{PG}\|_2 \leq (1+\Lambda) \min_{\bar{\boldsymbol{y}} \in \mathcal{ST}} \|\bar{\boldsymbol{y}} - \bar{\boldsymbol{w}}_{PG}\|_2$$

+ Linear Lebesgue constant growth in time

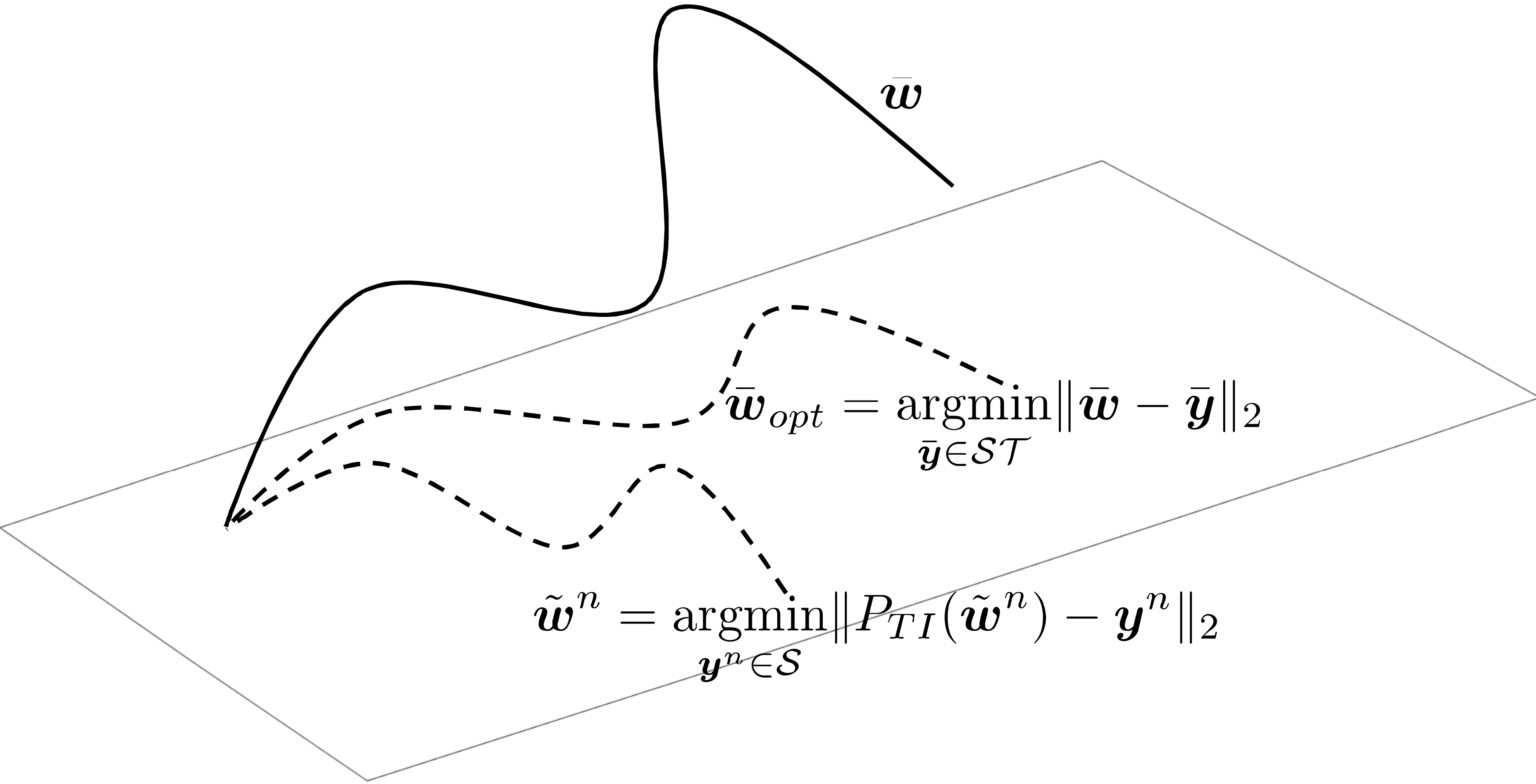
Lebesgue constant, Λ

$$\Lambda := \frac{\sigma_{\max}(\boldsymbol{A}_{LM}) - \sigma_{\min}(\boldsymbol{A}_{LM}) + 2\Delta t L_f \sigma_{\max}(\boldsymbol{B}_{LM})}{\sigma_{\min}(\boldsymbol{A}_{LM}) - \Delta t L_f \sigma_{\max}(\boldsymbol{B}_{LM})}$$



- Backward Euler (BE)
- Backward differentiation formulas (BDF2, BDF3)
- Adams-Bashforth (AB2, AB3)
- Adams-Moulton (AM1, AM2, AMD3)

Interpretation of error bound



1D Burgers' equation

- The governing equation

$$\frac{\partial w(x,t)}{\partial t} + \frac{\partial f(w(x,t))}{\partial x} = 0.02e^{\mu_2 x}$$

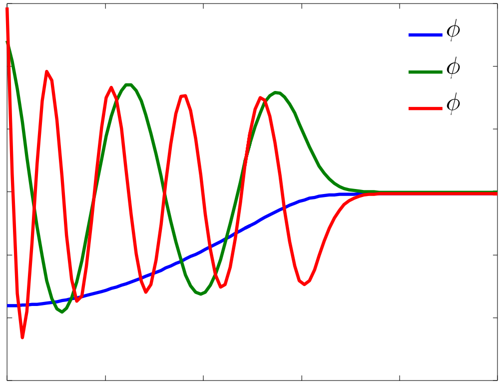
$$w(0,t) = \mu_1$$

$$w(x,0) = 1$$

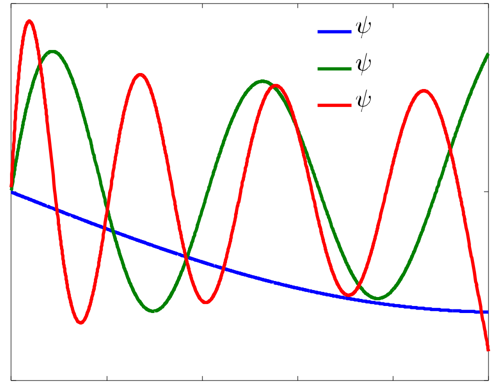
where $w \in \mathbb{R}$ for all $t \in [0, 0.5]$ and $x \in [0, 1]$

- Spatial discretization : a finite volume method, $\Delta x = 0.01$
- Time integrator : the Backward Euler method, $\Delta t = 2.5 \times 10^{-4}$
- Parameter, $\boldsymbol{\mu} \in \mathcal{D} = [1.2, 1.5] \times [0.02, 0.025]$
- Training set, $\mathcal{D}_{\text{train}} = \{1.2, 1.3, 1.4, 1.5\} \otimes \{0.02, 0.025\}$

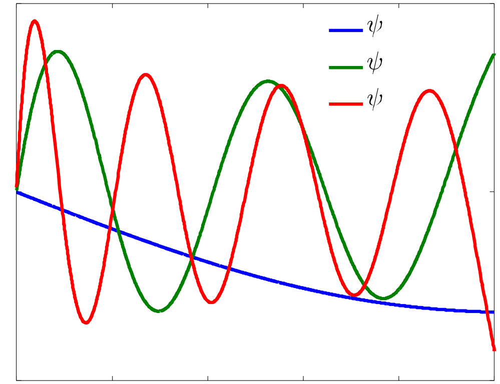
Space and time bases



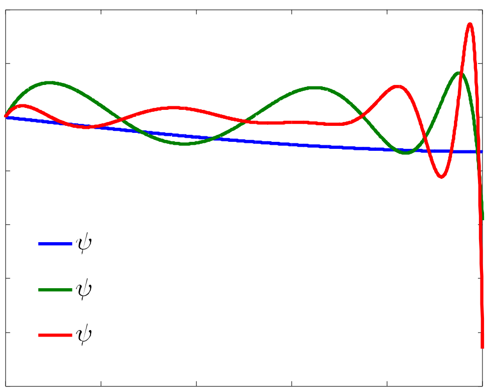
(a) Spatial basis



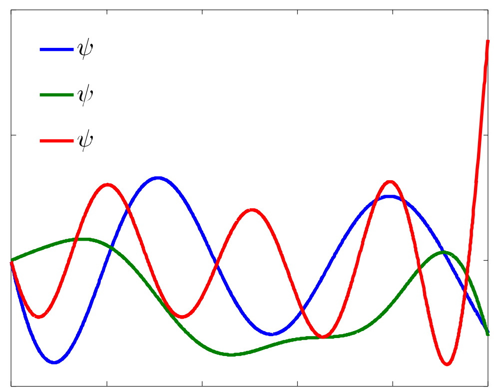
(b) Fixed temporal basis, T-HOSVD



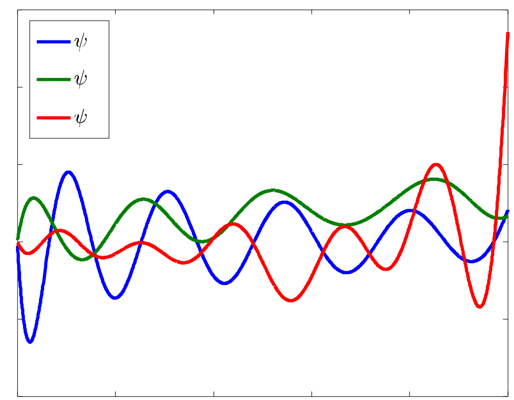
(c) Fixed temporal basis, ST-HOSVD



(d) Tailored temporal basis for ϕ_1



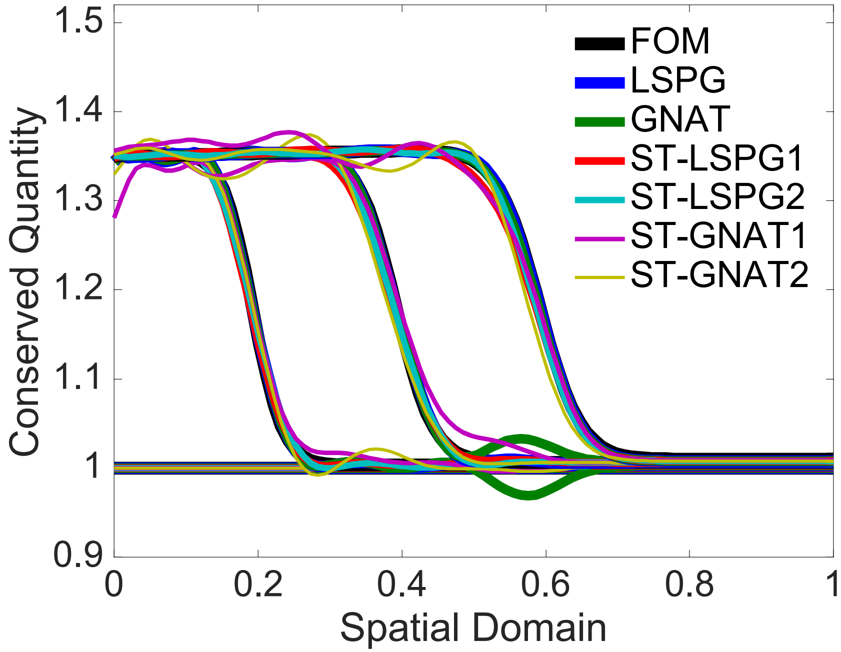
(d) Tailored temporal basis for ϕ_5



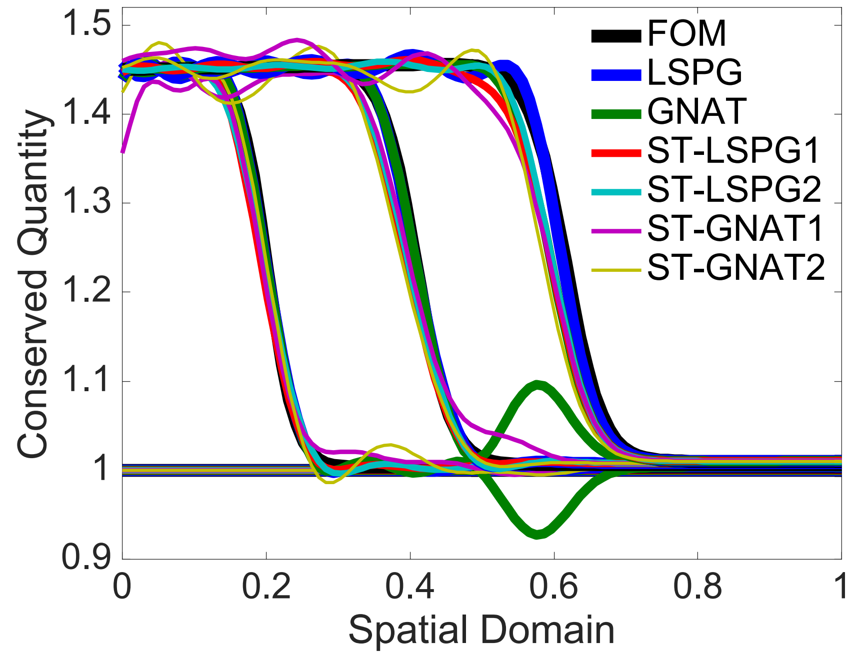
(d) Tailored temporal basis for ϕ_{10}

Solution history

$$\boldsymbol{\mu} = (1.35, 0.0229) \notin \mathcal{D}_{\mathrm{train}}$$



$$\boldsymbol{\mu} = (1.45, 0.0201) \notin \mathcal{D}_{\mathrm{train}}$$



Accuracy and speedup

$$\boldsymbol{\mu} = (1.35, 0.0229) \notin \mathcal{D}_{\text{train}}$$

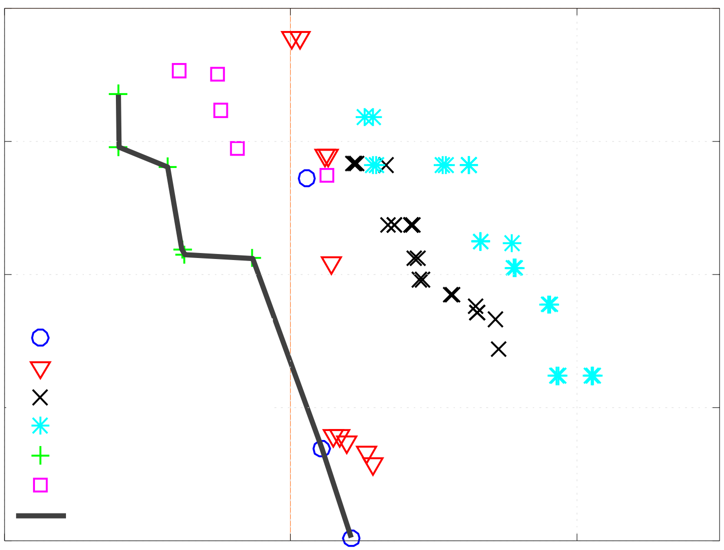
Method	LSPG	GNAT	ST-LSPG1	ST-LSPG2	ST-GNAT1	ST-GNAT2
Rel. Error	0.0027	0.0098	0.0051	0.0043	0.0093	0.0087
Speedup	0.86	0.80	0.25	0.031	**4.73**	2.59

$$\boldsymbol{\mu} = (1.45, 0.0201) \notin \mathcal{D}_{\text{train}}$$

Method	LSPG	GNAT	ST-LSPG1	ST-LSPG2	ST-GNAT1	ST-GNAT2
Rel. Error	0.0042	0.015	0.012	0.011	0.016	0.017
Speedup	0.76	1.04	0.40	0.039	**9.96**	3.15

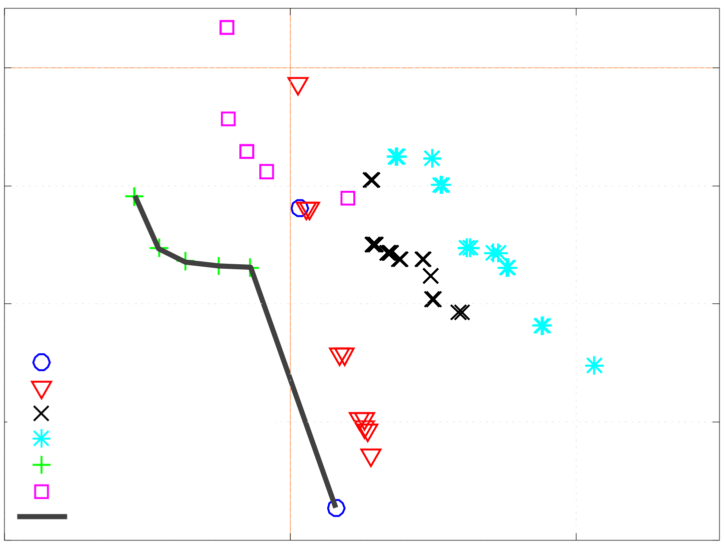
Pareto fronts

$\boldsymbol{\mu} = (1.35, 0.0229) \notin \mathcal{D}_{\text{train}}$



Slowdown

$\boldsymbol{\mu} = (1.45, 0.0201) \notin \mathcal{D}_{\text{train}}$



Slowdown

Conclusion

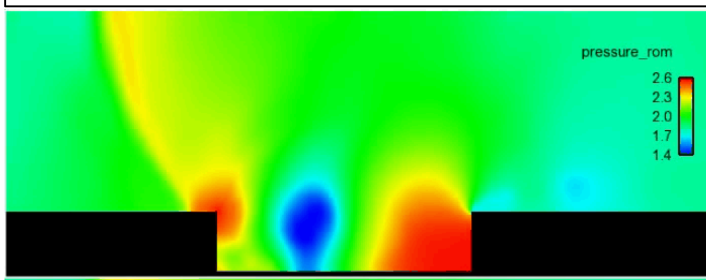
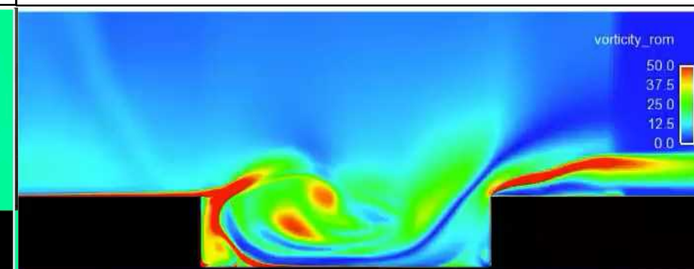
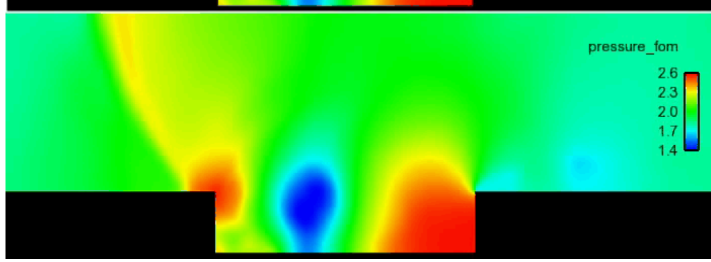
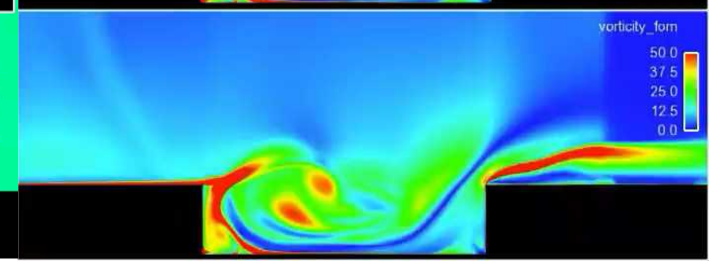
Accomplishment

+ Complexity is independent of both space and time
+ Construction is purely algebraic
+ Does not require a space–time full-order model
+ Amenable to any time integrator
+ Slower time growth in error bound

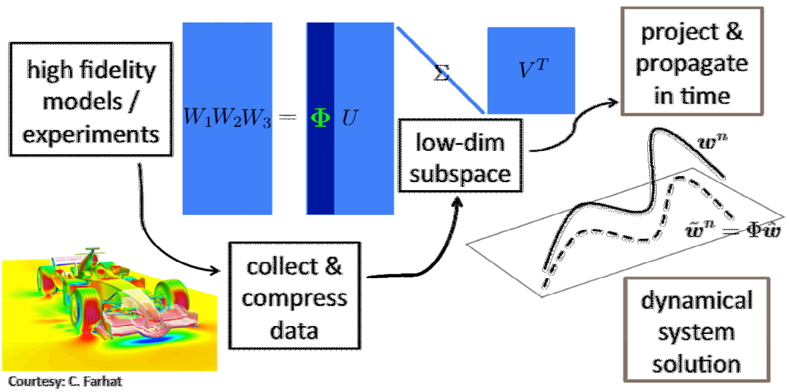
Future work

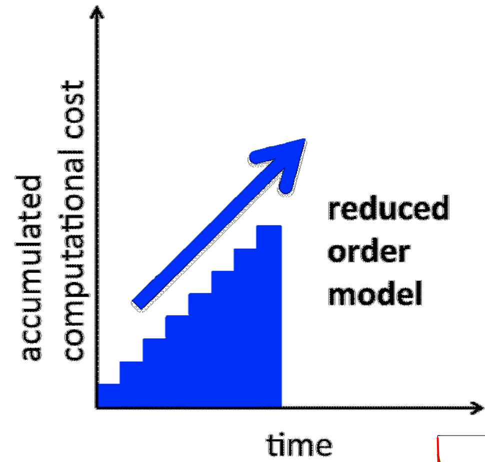
- Implement in high performance computing codes
- Apply the method in PDE-constrained optimization and UQ

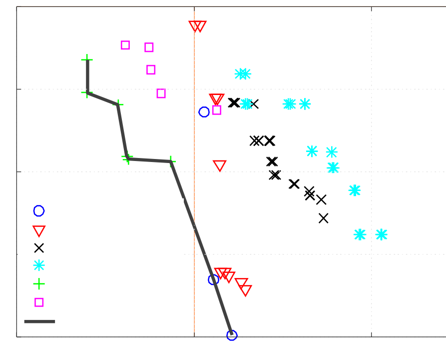
Captive-carry simulation

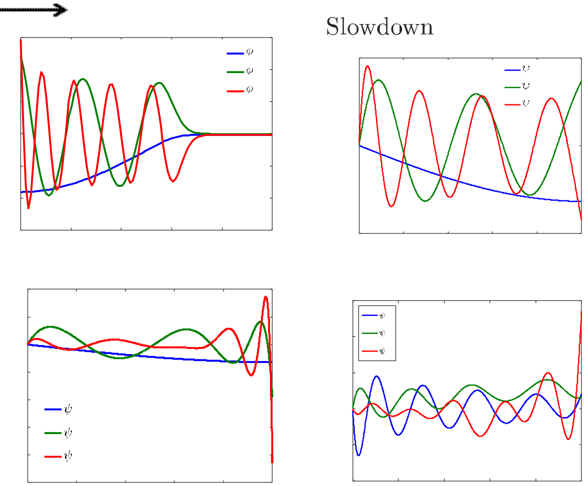
	Pressure field	Vorticity field
GNAT-ST ? min, ? cores	?	?
GNAT ROM 32 min, 2 cores Courtesy: K. Carlberg		
High-fidelity 5 hours, 48 cores Courtesy: M. Barone		

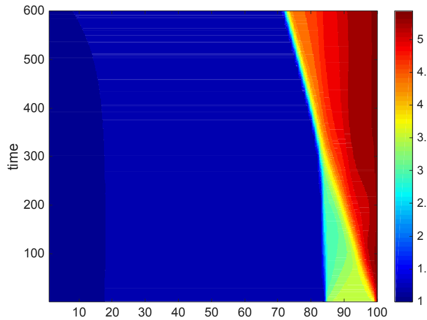
Questions

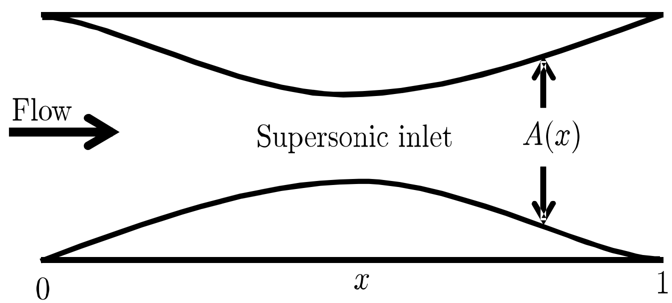






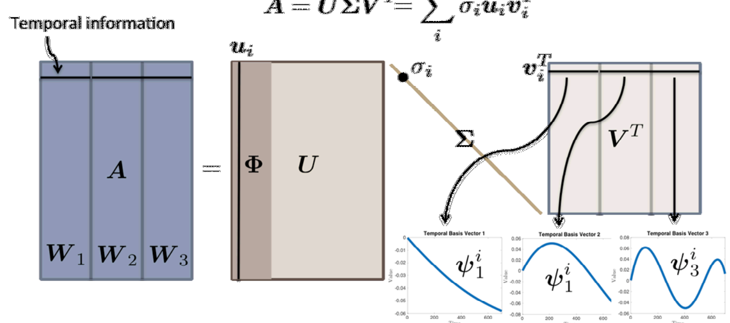






Singular value decomposition

$$A = U\Sigma V^T = \sum_i \sigma_i u_i v_i^T$$



Tailored temporal basis