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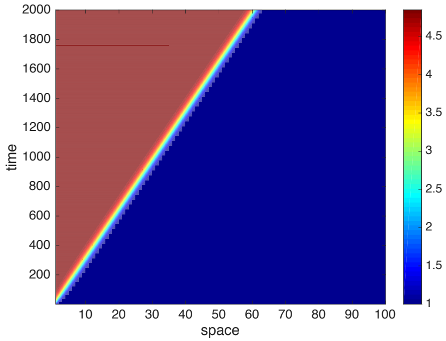
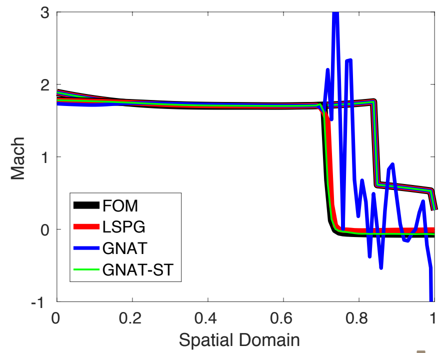
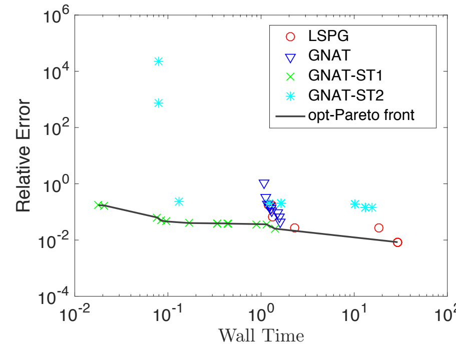
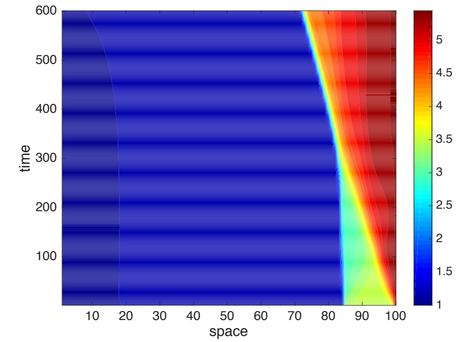








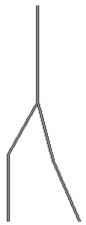
Space-time least-squares Petrov-Galerkin nonlinear model reduction

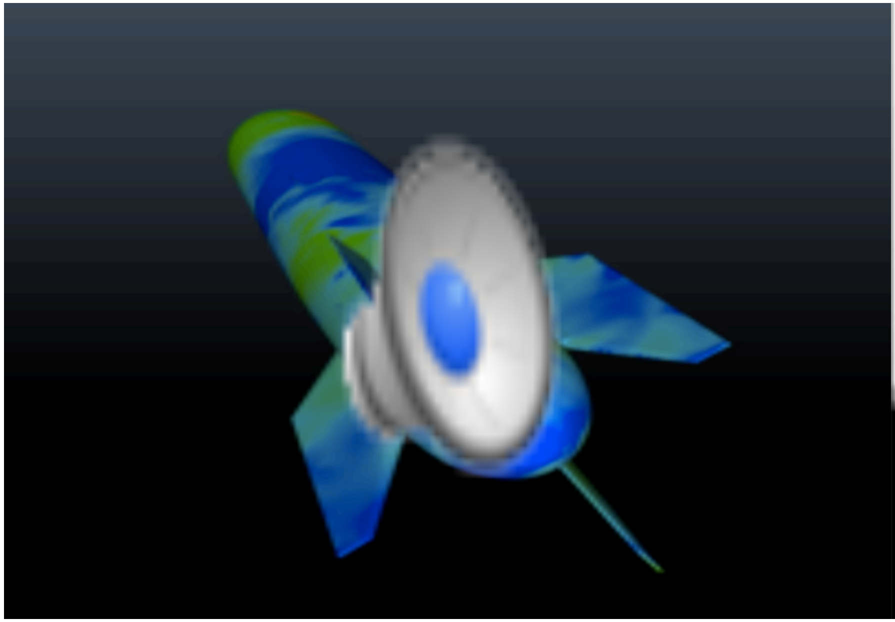
Youngsoo Choi and Kevin Carlberg

U.S. DEPARTMENT OF ENERGY

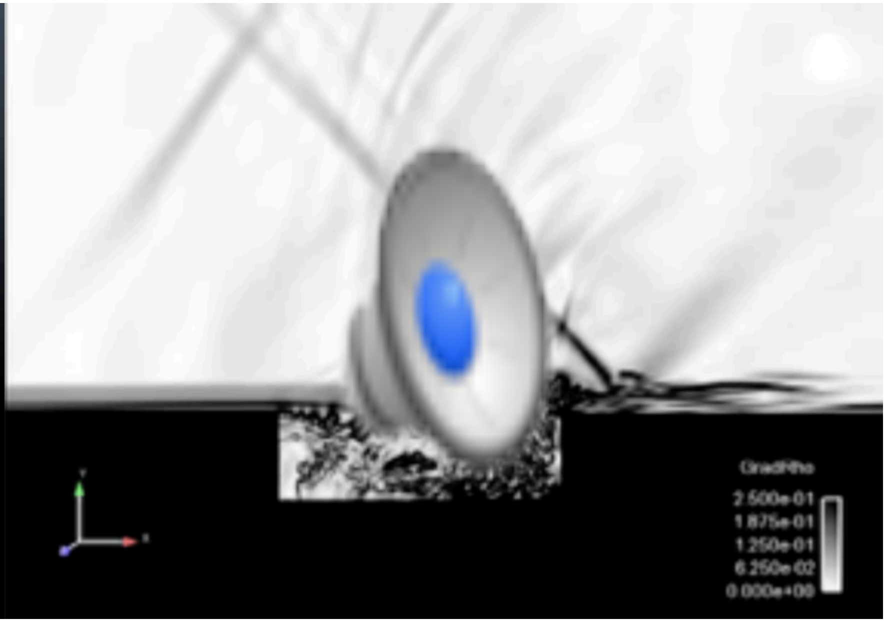
NNSA National Nuclear Security Administration

Nonlinear Dynamical Simulation





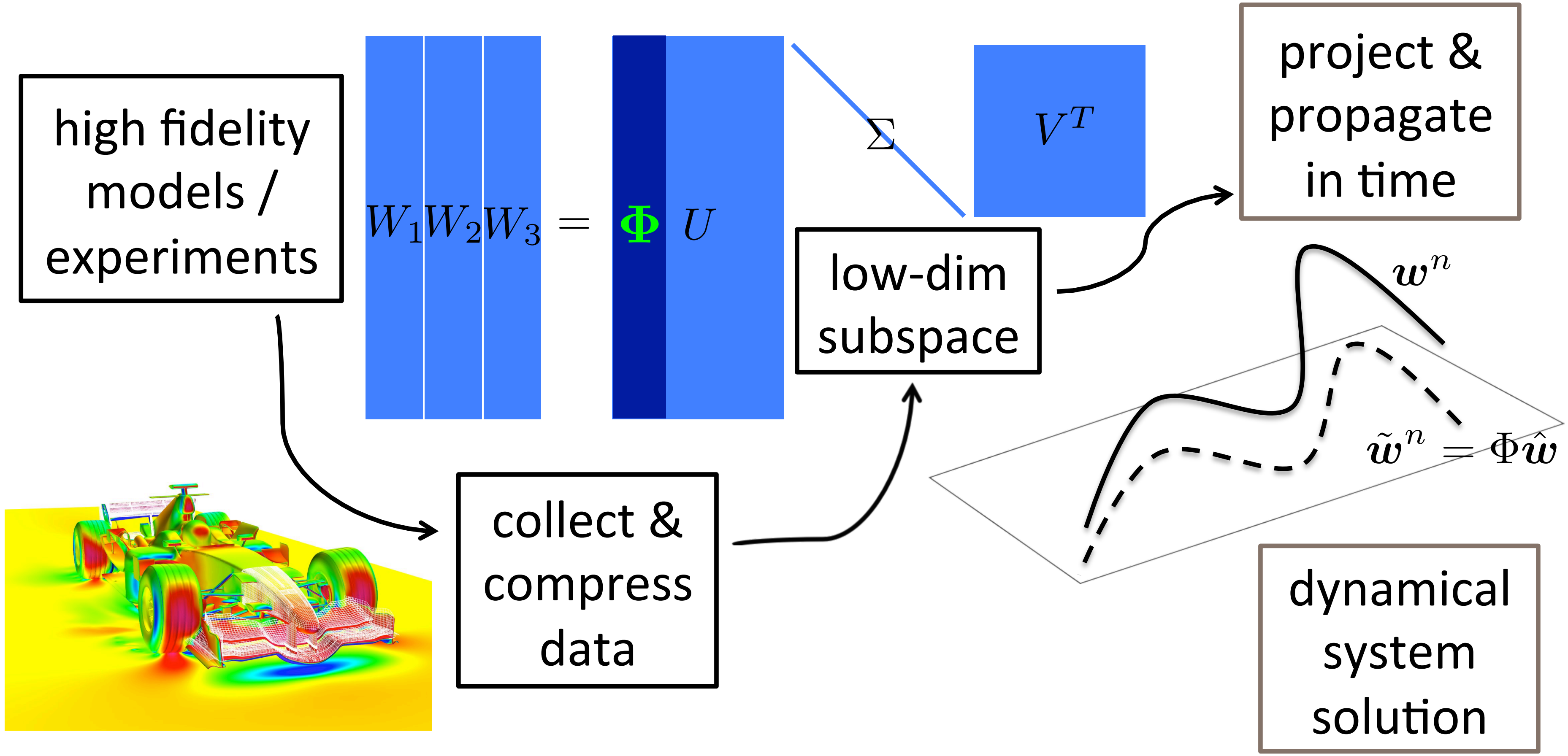
Courtesy: K. Carlberg



Courtesy: K. Carlberg

Reduced Order Model (ROM)

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



ROM often works very well

Physical data are strongly correlated due to physical laws

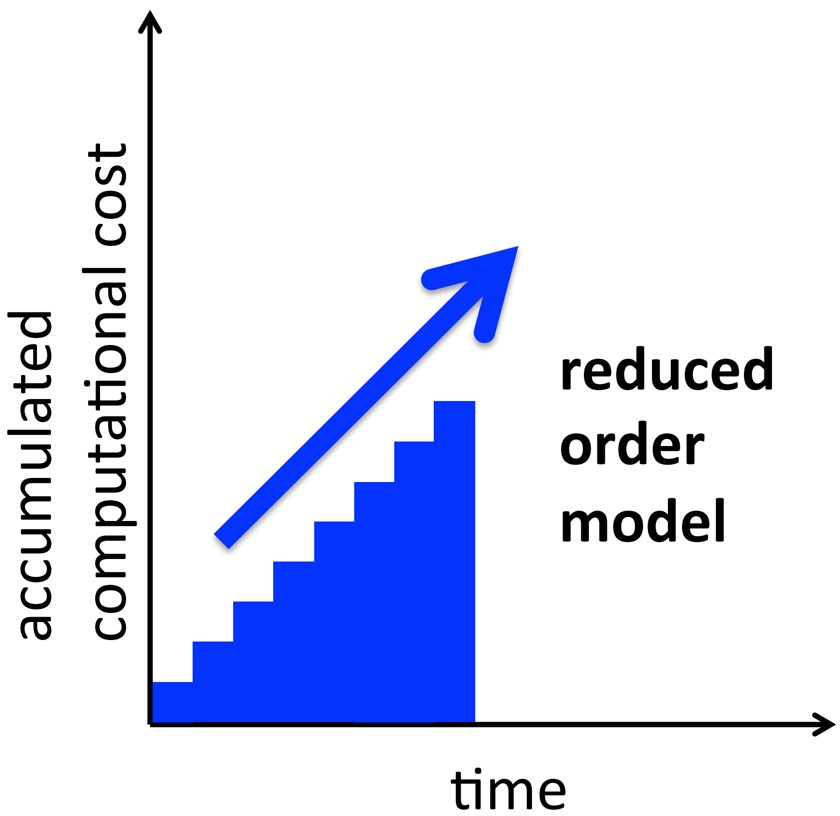
↓

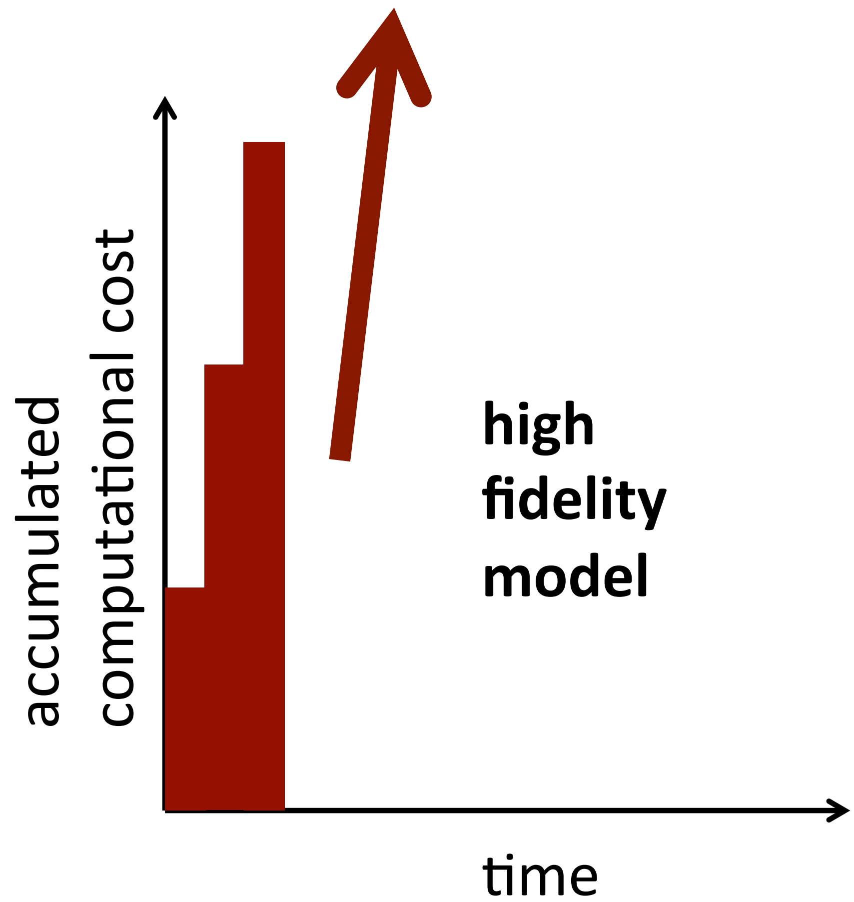
Redundancies in space and time

↓

Restriction of solution onto a subspace with small dimension keeps accuracy high enough

Complexity in time



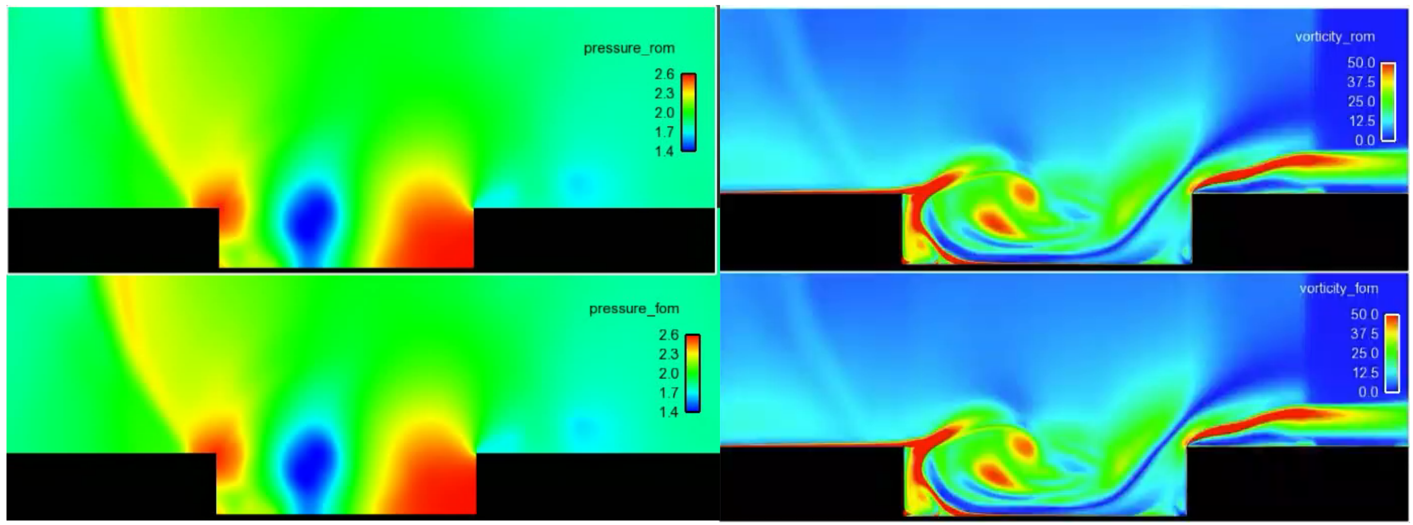


Captive-carry simulation

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

Outline

- Full order models
- A typical projection-based ROM
- A space–time ROM

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- A space–time ROM

A system of nonlinear ODEs

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

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

Fully discrete system, OΔE

Linear multistep schemes

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

- Uniform time step: Δt
- Total time steps: $N_t := T/\Delta t \in \mathbb{N}$
- $n \in \mathbb{N}(N_t)$

At *n*th time step, solve $\boldsymbol{r}^n(\boldsymbol{w}^n) = \boldsymbol{0}$

The Newton method

***j*th Newton step at *n*th time step**

$$\boldsymbol{J}_j^n \Delta \boldsymbol{w}_j = \boldsymbol{r}_j^n$$

$$\boldsymbol{w}_{j+1}^n \leftarrow \boldsymbol{w}_j^n + \Delta \boldsymbol{w}_j$$

- States, $\boldsymbol{w}_j^n, \boldsymbol{w}_{j+1}^n \in \mathbb{R}^{N_s}$
- Increment, $\Delta \boldsymbol{w}_j \in \mathbb{R}^{N_s}$
- Residual, $\boldsymbol{r}_j^n := \boldsymbol{r}^n(\boldsymbol{w}_j^n) \in \mathbb{R}^{N_s}$
- Jacobian, $\boldsymbol{J}_j^k := \nabla \boldsymbol{r}^n(\boldsymbol{w}_j^n) \in \mathbb{R}^{N_s \times N_s}$

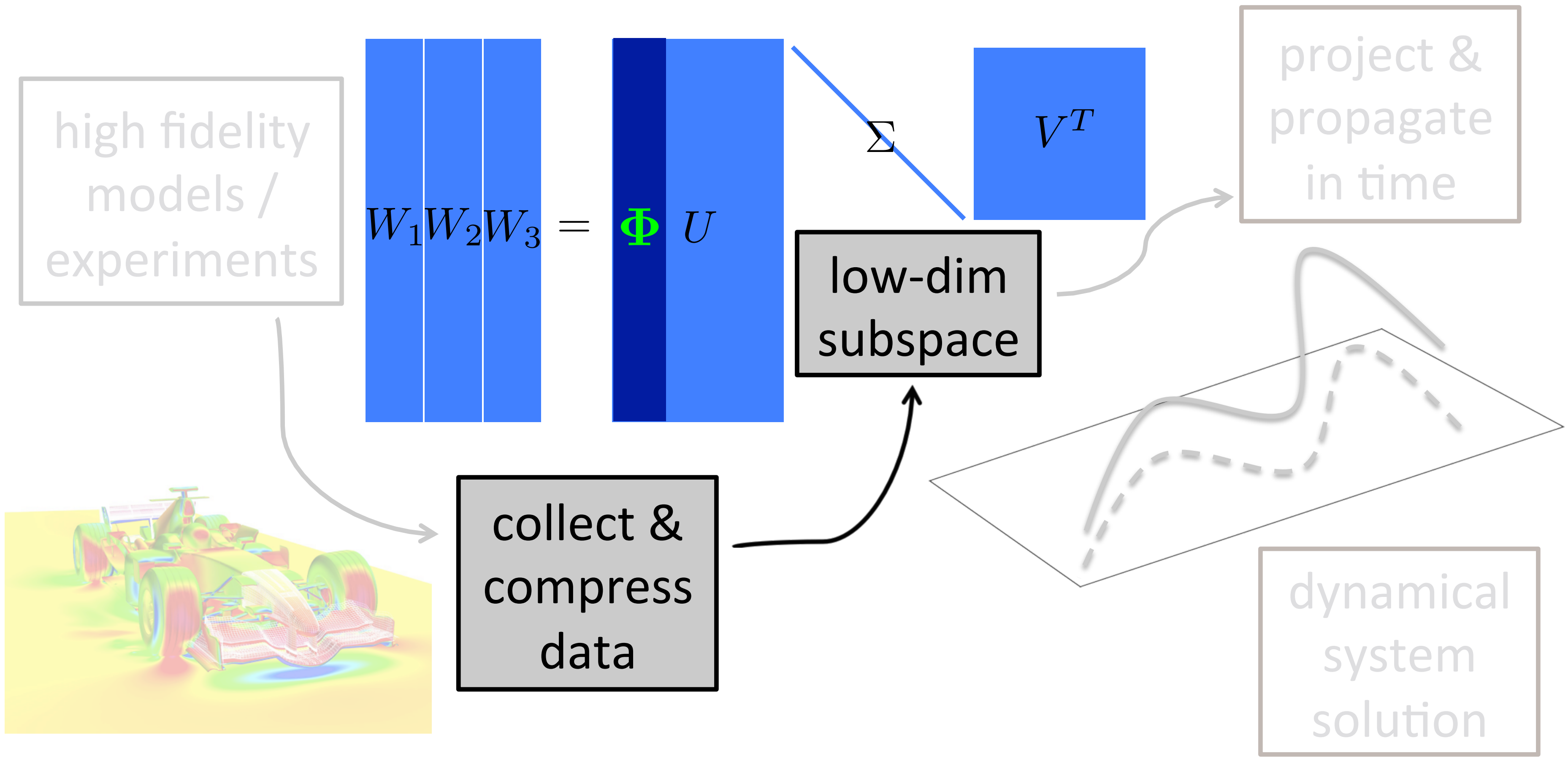
Costly:

- State dimension
- Residual size
- Jacobian size
- A large system of equations to solve

Outline

- Full order models
- A typical projection-based ROM
- A space–time ROM

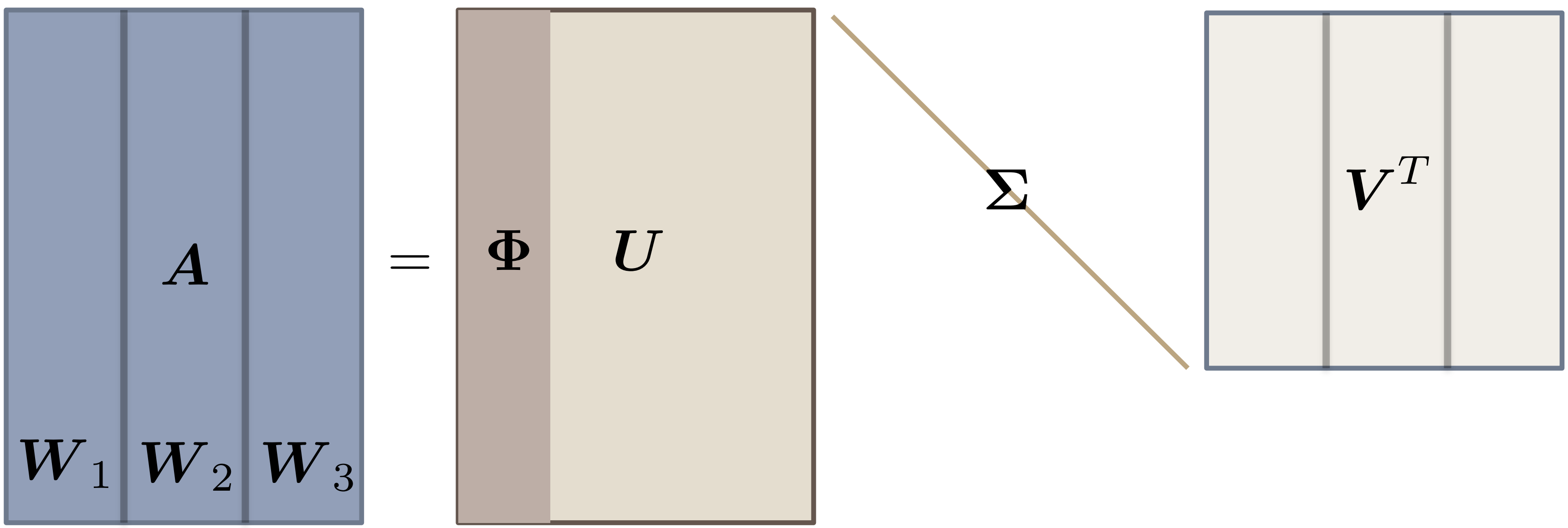
Subspace generation



Subspace generation

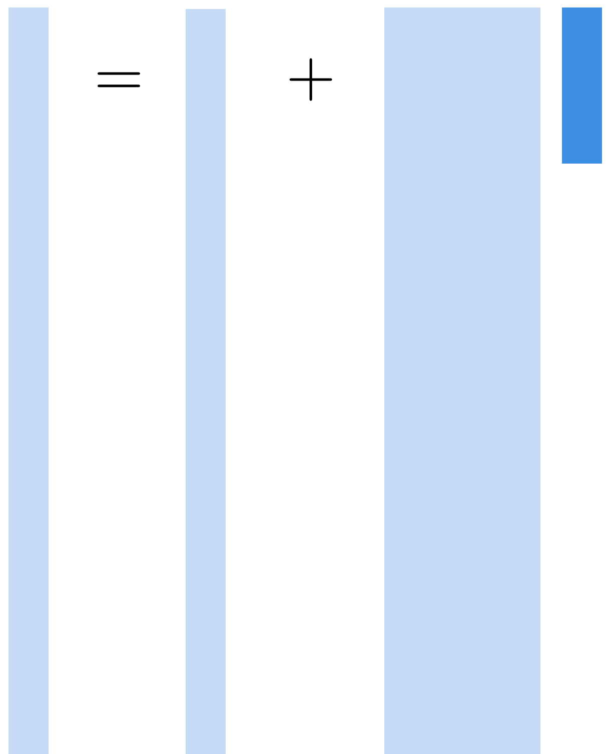
Singular value decomposition

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



State approximation

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



Spatiotemporal subspace

$$\tilde{\boldsymbol{w}} \in \boldsymbol{w}_{ref} \otimes \mathbf{1}_{N_t} + \mathcal{S} \otimes \mathbb{R}^{N_t} \subseteq \mathbb{R}^{N_s} \otimes \mathbb{R}^{N_t}$$

$$\Updownarrow$$

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

- 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

Projection

Over-determined nonlinear system

$$\boldsymbol{r}^n(\boldsymbol{w}_{ref} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}^n) = \mathbf{0}$$

- Unknowns, $\hat{\boldsymbol{w}} := \hat{\boldsymbol{w}}(t^n) \in \mathbb{R}^{n_s}$
- Equations, $\boldsymbol{r}^n \in \mathbb{R}^{N_s}$

Two projections

- Galerkin, $\boldsymbol{\Phi}^T \boldsymbol{r}^n(\boldsymbol{w}_{ref} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}^n) = \mathbf{0}$
- Petrov-Galerkin, $\boldsymbol{\Lambda}^T \boldsymbol{r}^n(\boldsymbol{w}_{ref} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}^n) = \mathbf{0}$

$$\boldsymbol{\Lambda}, \boldsymbol{\Phi} \in \mathbb{R}^{N_s \times n_s}, \quad \boldsymbol{\Lambda} \neq \boldsymbol{\Phi}$$

Least-squares Petrov-Galerkin projection

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: $\boldsymbol{G} = (\boldsymbol{Z}\boldsymbol{\Phi}_r)^\dagger \boldsymbol{Z} \in \mathbb{R}^{n_r \times N_s}$

⬆

$$\underset{\hat{\boldsymbol{r}}}{\text{minimize}} \quad \|\boldsymbol{Z}(\boldsymbol{r} - \boldsymbol{\Phi}_r \hat{\boldsymbol{r}})\|_2^2$$

$\boldsymbol{r} =$

$\boldsymbol{Z}\boldsymbol{r} =$

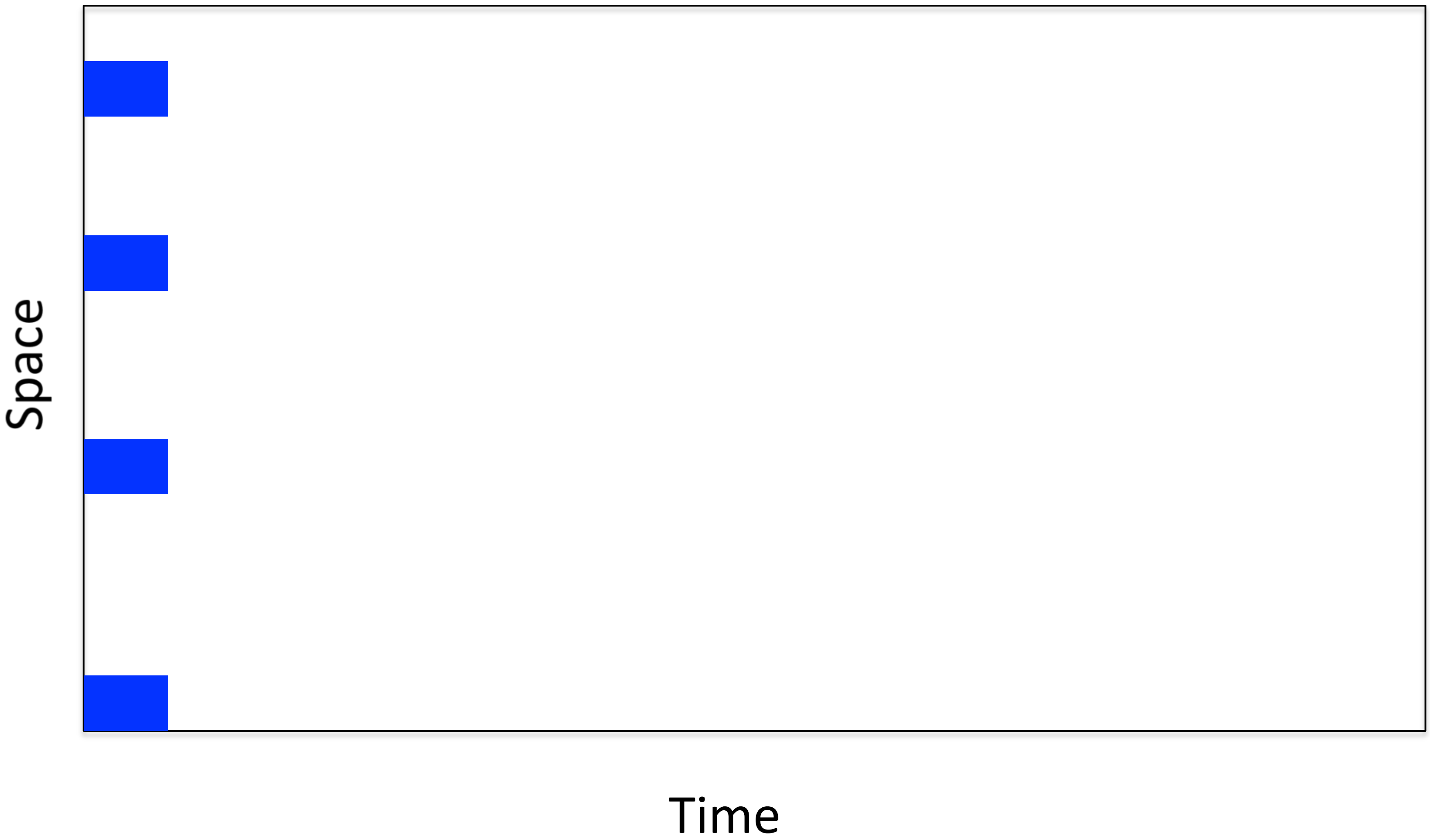
- Optimality condition

$$\boldsymbol{\Lambda}^T \boldsymbol{r}^n(\boldsymbol{w}_{ref} + \boldsymbol{\Phi}\hat{\boldsymbol{w}}^n) = \boldsymbol{0}$$

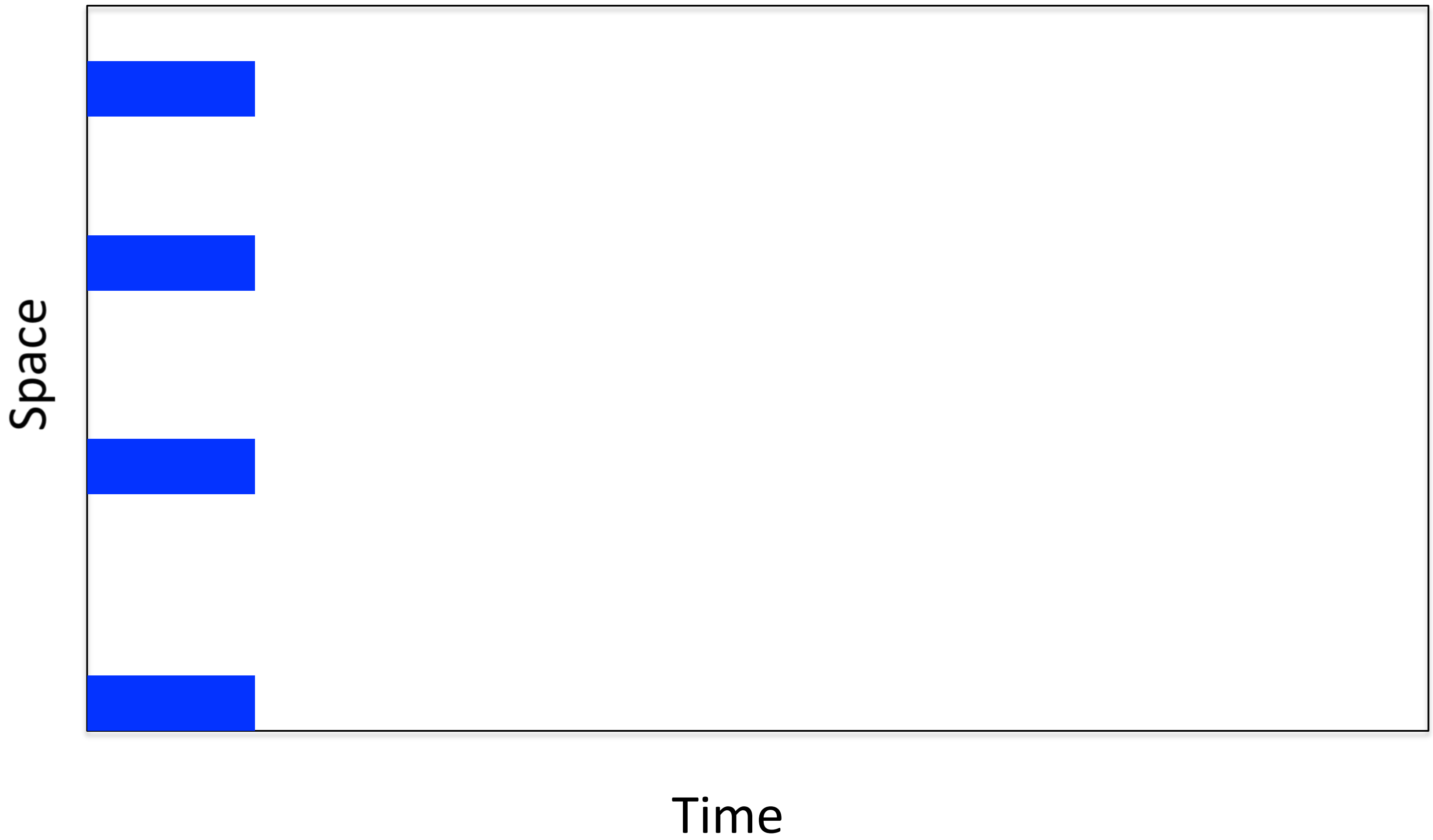
\+ Spatial complexity reduction achieved

– No temporal complexity reduction: N_t time steps

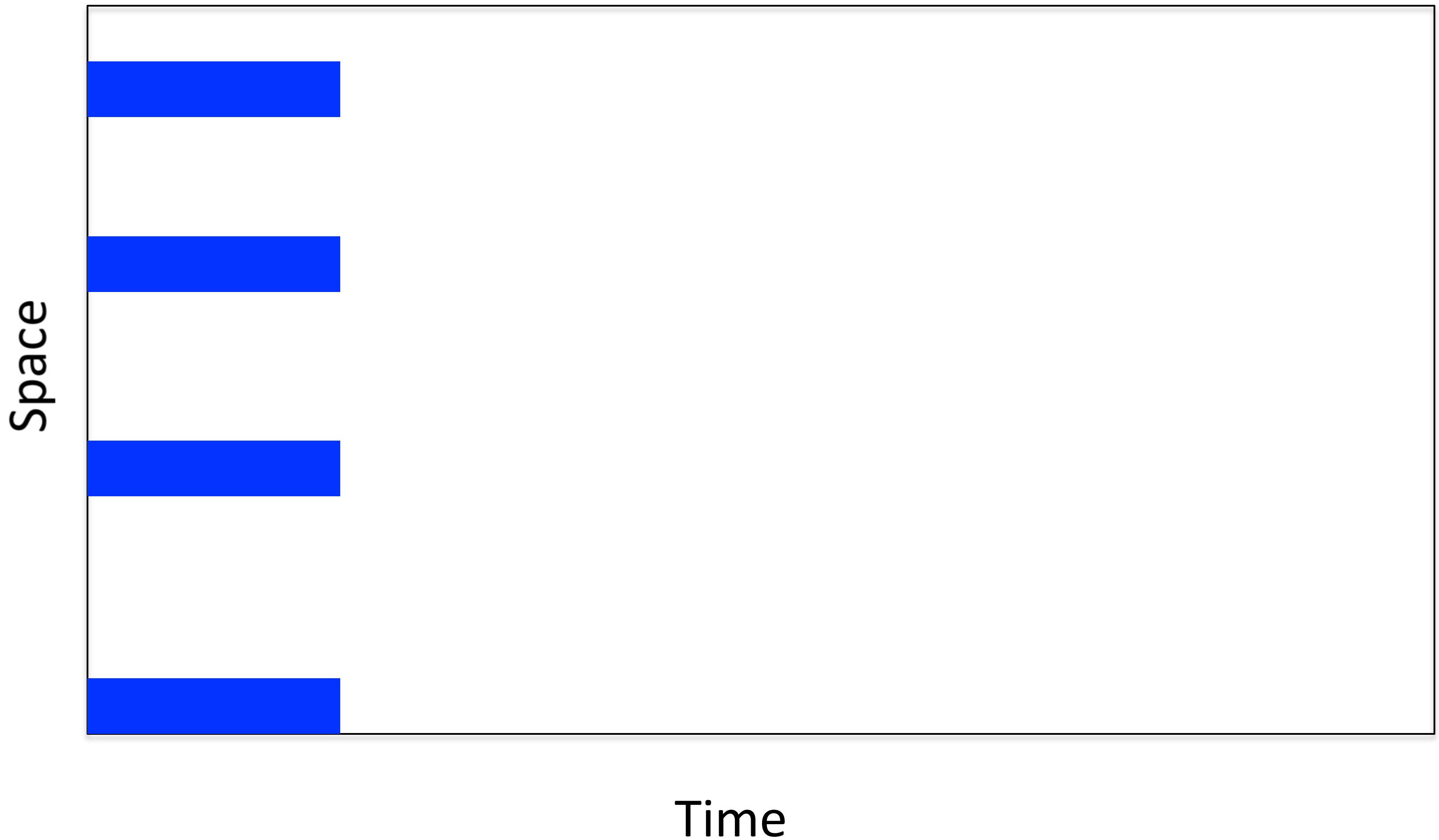
Complexity figure



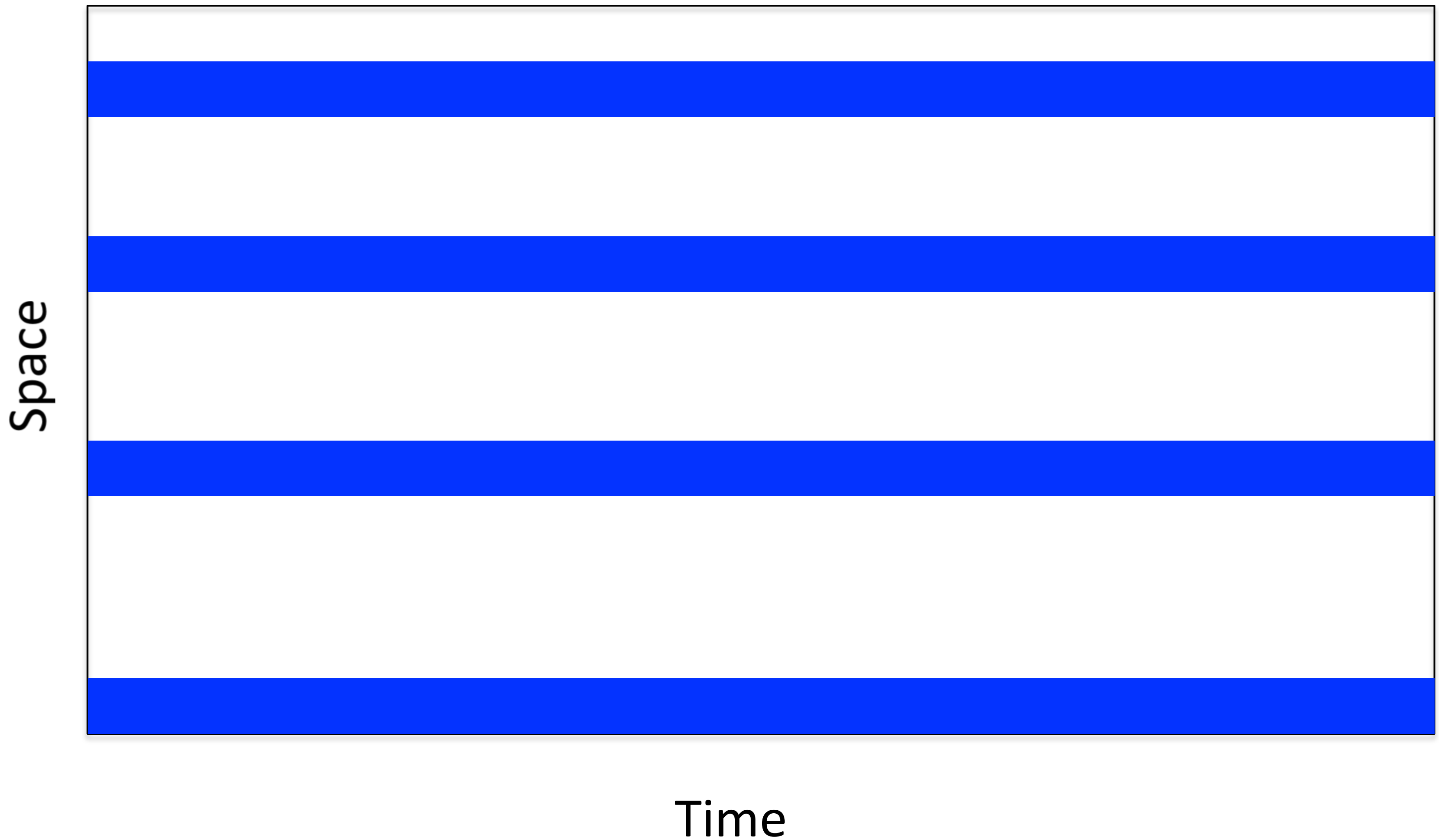
Complexity figure



Complexity figure



Complexity figure



Outline

- Full order models
- A typical projection-based ROM
- A space–time ROM

Motivation

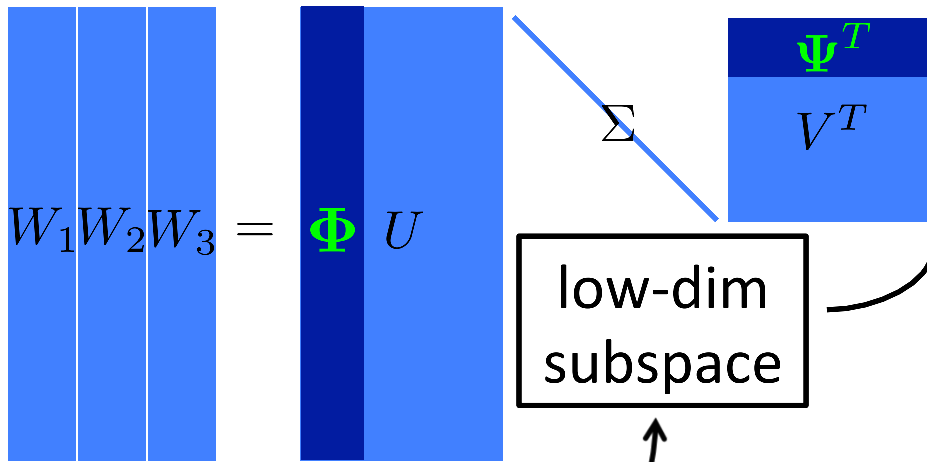
- Typical ROMs apply spatial projection
  - + Reduces spatial computational complexity
  - – Does not reduce temporal complexity (number of time steps remains large)
- Larger time steps with explicit time integration [Krysl et al., 2001]
  - + Larger stable time steps achievable with ROMs
  - – Speedup 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

Space–time ROM

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

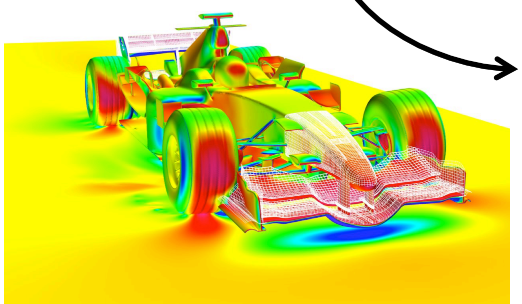
only once

high fidelity models / experiments



low-dim subspace

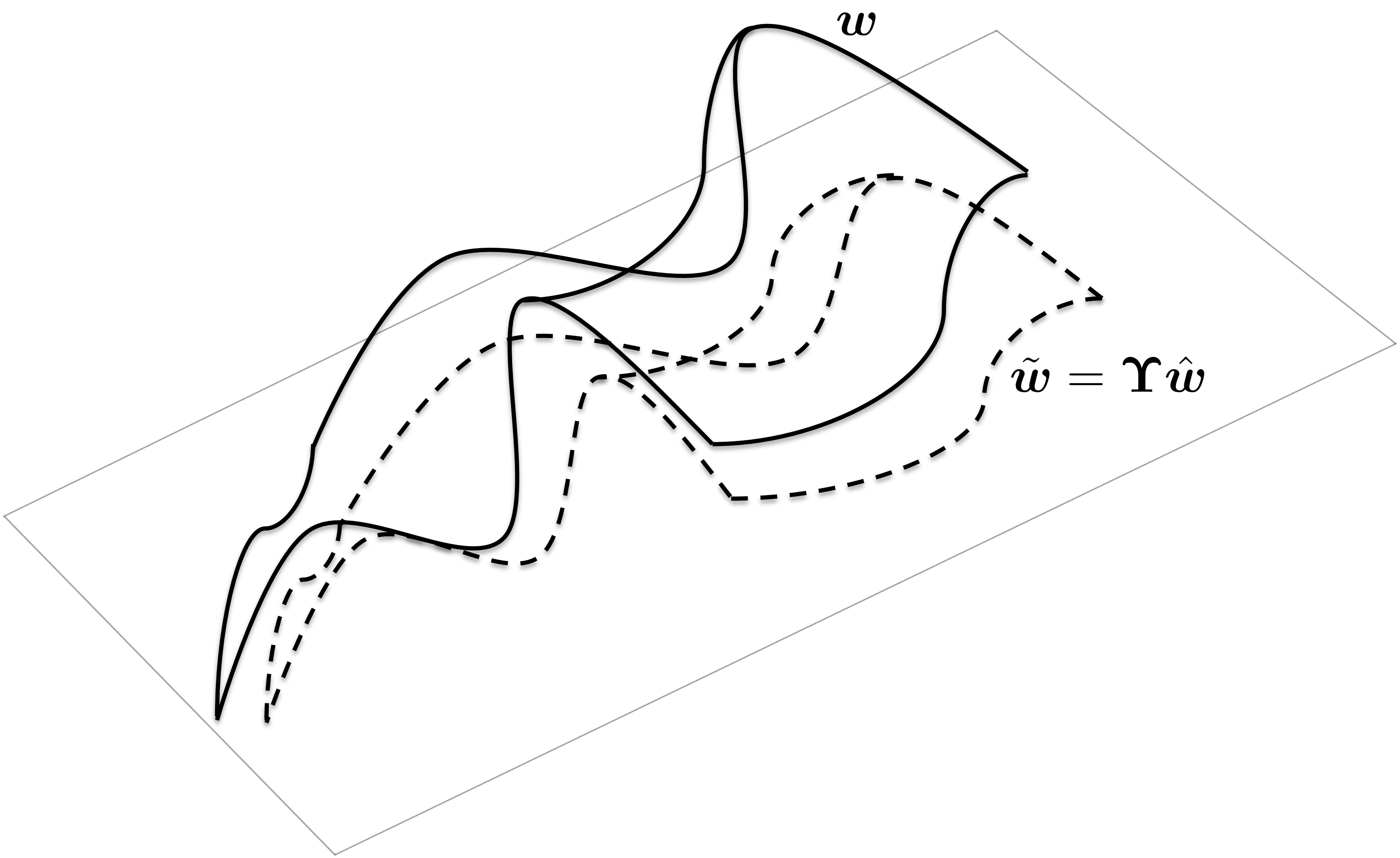
Space–time project



collect & compress data

dynamical system solution

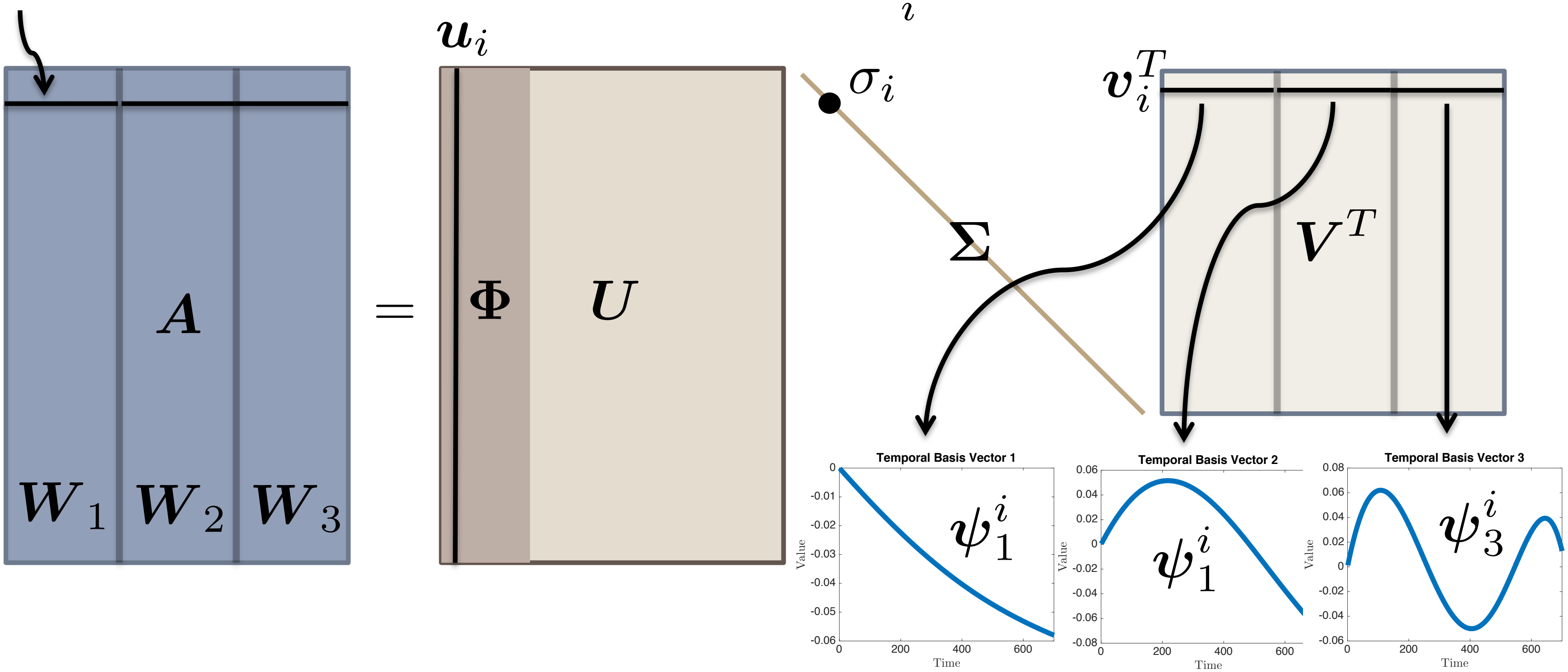
Space–time projection



Subspace generation I

Singular value decomposition

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

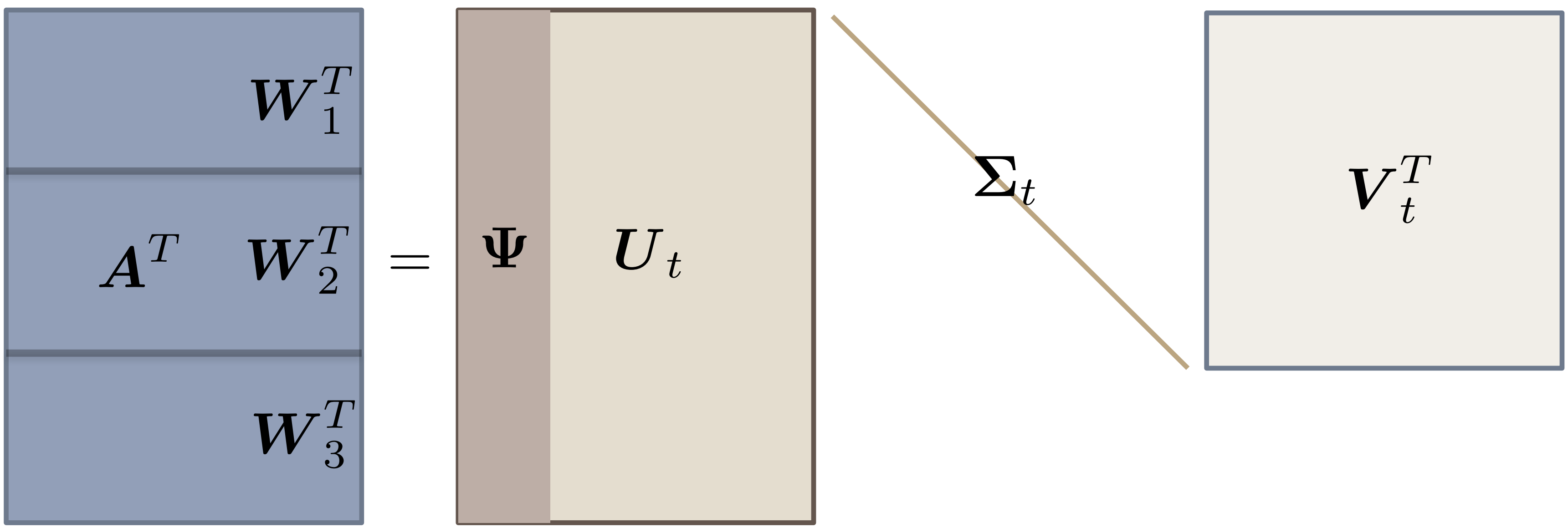


Tailored temporal basis

Fixed temporal basis

Singular value decomposition

$$A^T = U_t \Sigma_t V_t^T$$



Space–time state basis

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

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

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

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

Spatiotemporal subspace

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

$$\Updownarrow$$

$$\tilde{\boldsymbol{w}}(t^n) = \boldsymbol{w}_{ref} + \sum_{i=1}^{n_s} \sum_{j=1}^{n_t^i} \boldsymbol{\phi}_i \psi_{jn}^i \hat{w}_{ij}$$

- 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

Spatiotemporal LSPG projection

- discrete-residual minimization

$$\hat{\boldsymbol{w}}_{\mathrm{st}} = \arg\min_{\hat{\boldsymbol{y}}} \left\| \sum_{n=1}^{N_t} \overline{\boldsymbol{G}}^n \boldsymbol{r}^n \left(\boldsymbol{w}_{ref} + \sum_{i=1}^{n_s} \sum_{j=1}^{n_t^i} \boldsymbol{\phi}_i \psi_{jn}^i \hat{y}_{ij}\right) \right\|_2^2$$

- LSPG: $\overline{\boldsymbol{G}}^n = \boldsymbol{I}$
- Collocation: $\overline{\boldsymbol{G}}^n = \overline{\boldsymbol{Z}}$
- GNAT: $\overline{\boldsymbol{G}}^n$ = *n*th column block of $(\overline{\boldsymbol{Z}\boldsymbol{\Phi}_r})^{\dagger}\overline{\boldsymbol{Z}}$

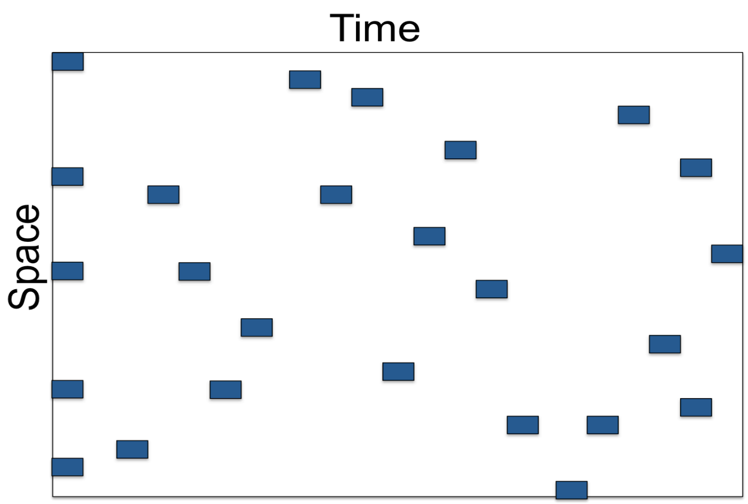
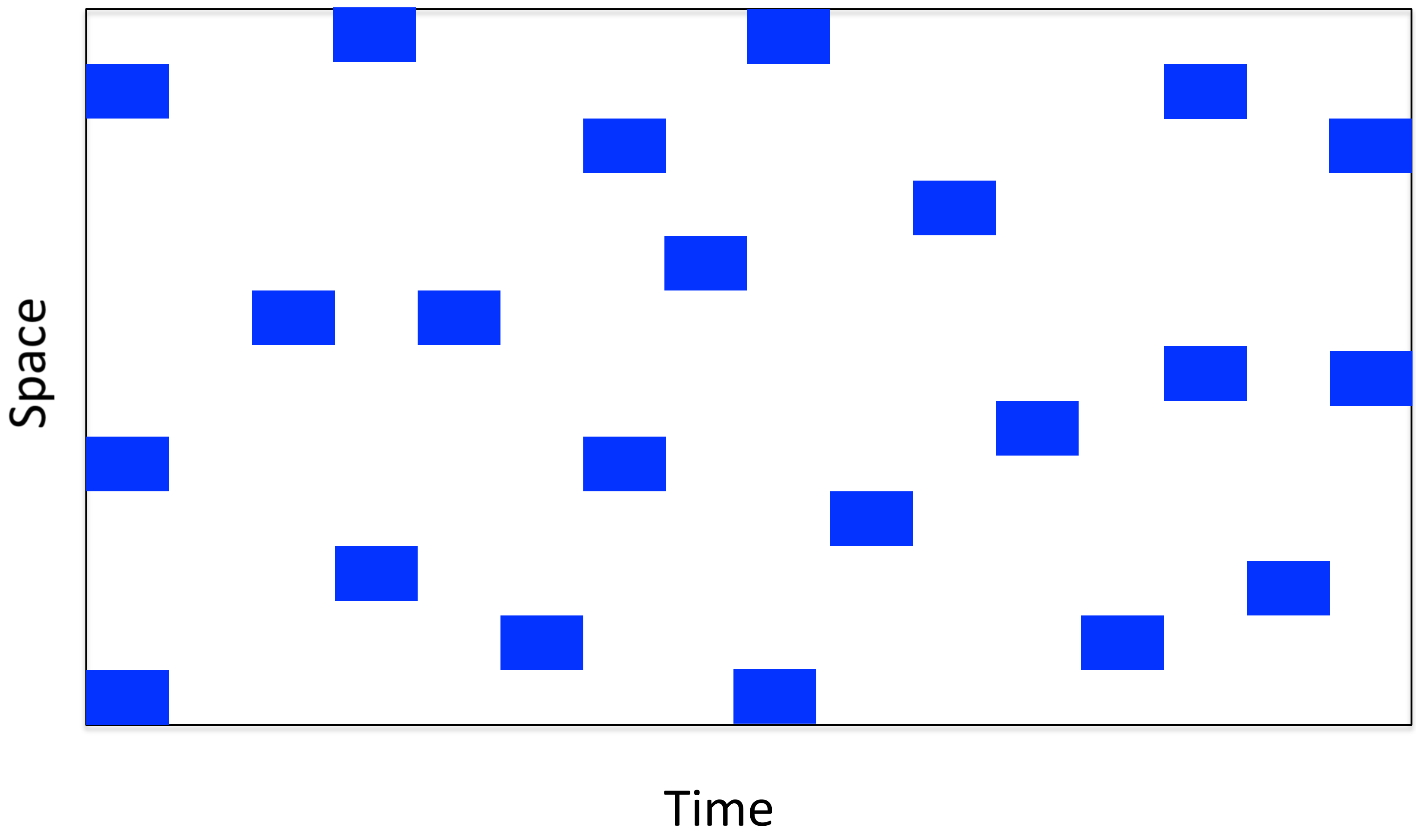


Figure: Spatiotemporal GNAT $\overline{Z}$

+ More complexity reduction

Complexity figure



Error bound

Spatial LSPG

- Linear multistep time integration [Carlberg et al., 2016]

$$\|\boldsymbol{w}_\star^n - \boldsymbol{w}_{PG}^n\|_2 \leq \sum_{j=0}^{n-1} \frac{\Delta t}{(h)^{j+1}} \|(\boldsymbol{I} - \mathbb{P}^{n-j})\boldsymbol{f}(\tilde{\boldsymbol{w}}_{PG}^{n-j})\|_2$$

− Exponential growth in time

Spatiotemporal LSPG

- Linear multistep time integration

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

\+ Slower stability-constant growth in time

1D Burgers' Equation

- The governing equation

$$\frac{\partial w(x,t)}{\partial t} + \frac{\partial f(w(x,t))}{\partial x} = g(x)$$

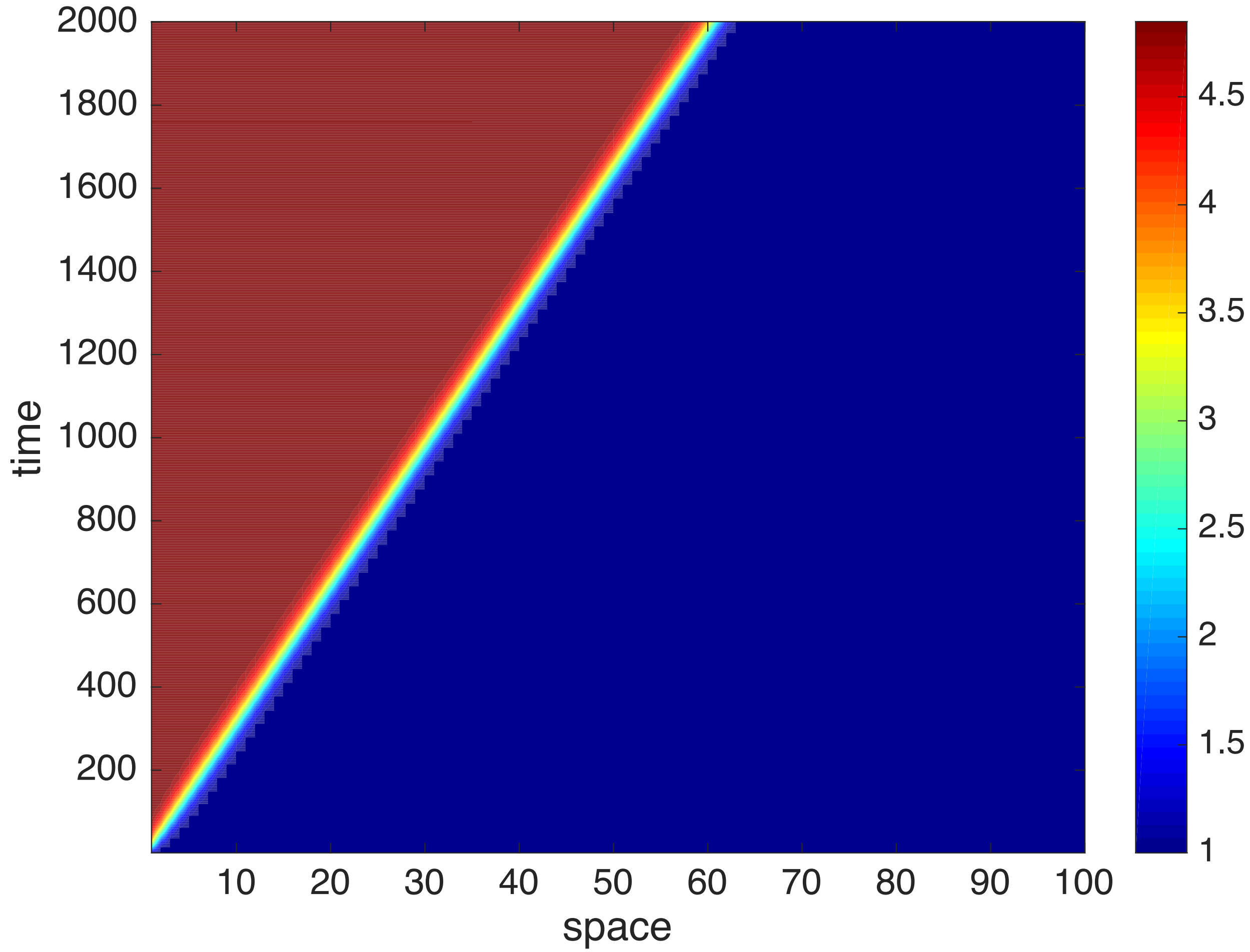
$$w(0,t) = \mu$$

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

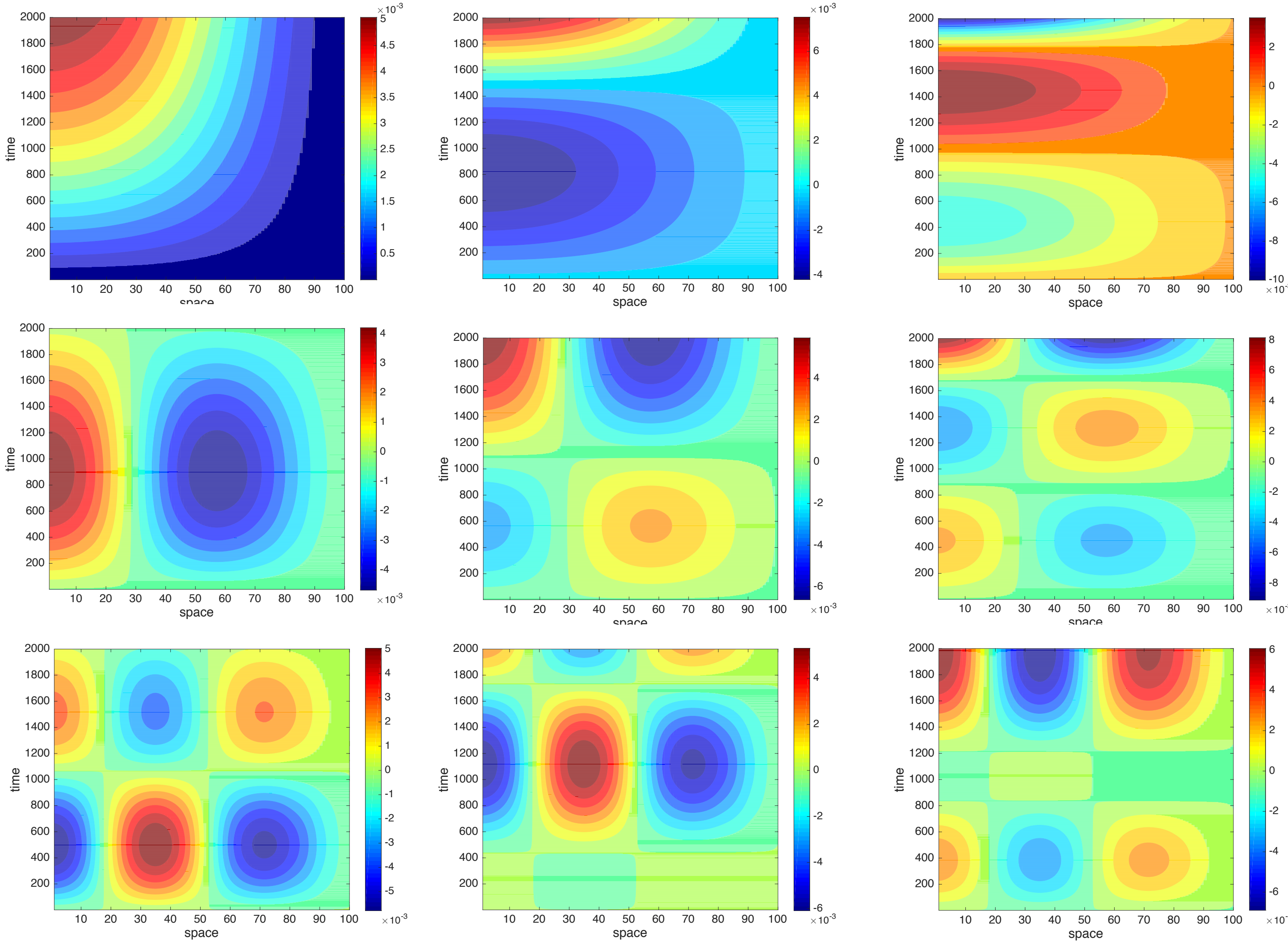
where $w \in \mathbb{R}$ for all $t > 0$ and $x \in [0,1]$

- Spatial discretization : a finite volume method
- Time integrator : the Backward Euler method

FOM solution

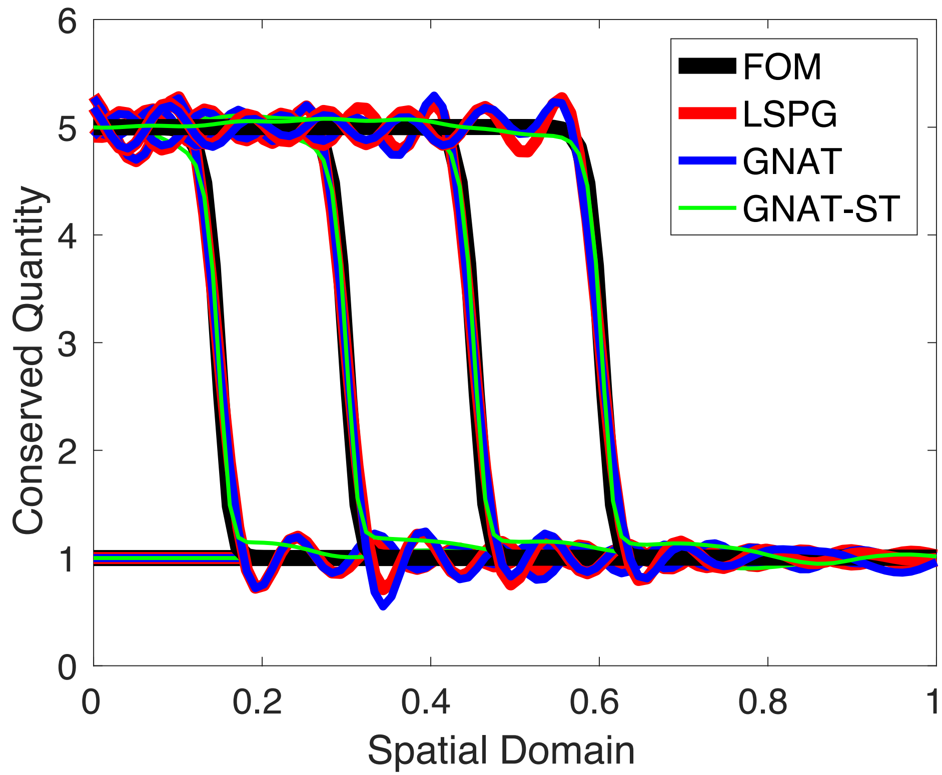


Spatiotemporal basis

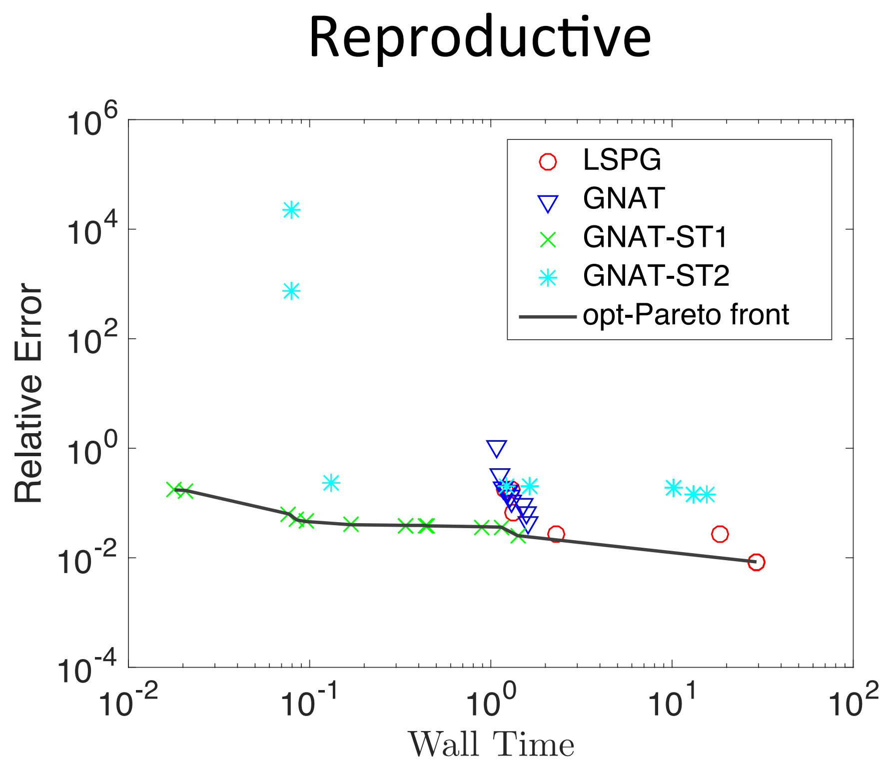


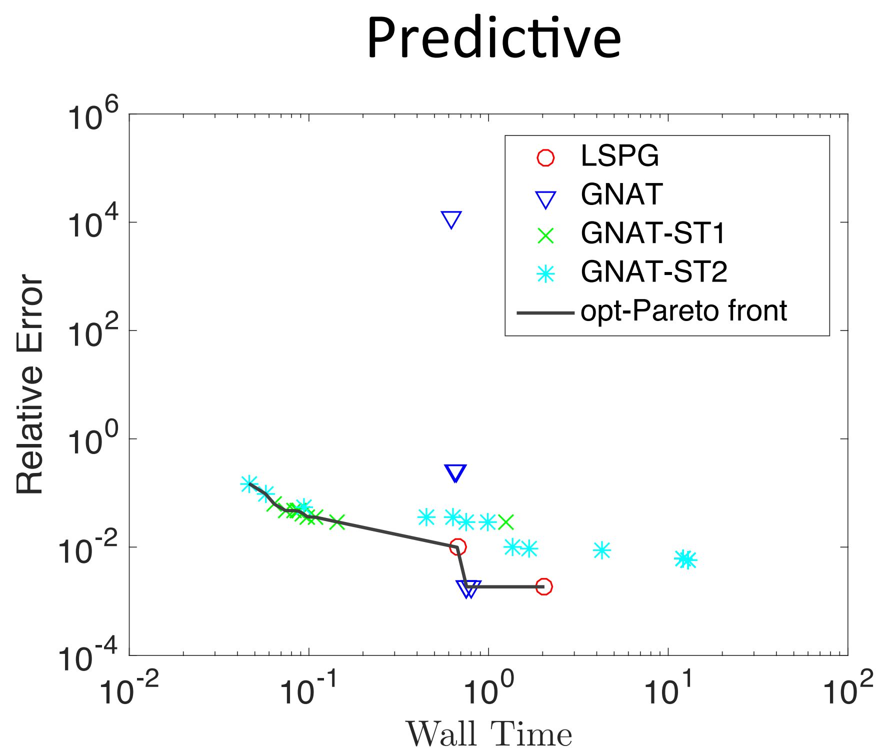
Solution History

- GNAT-ST is **10 times** faster than GNAT



Optimal Pareto front





Quasi 1D Euler equation

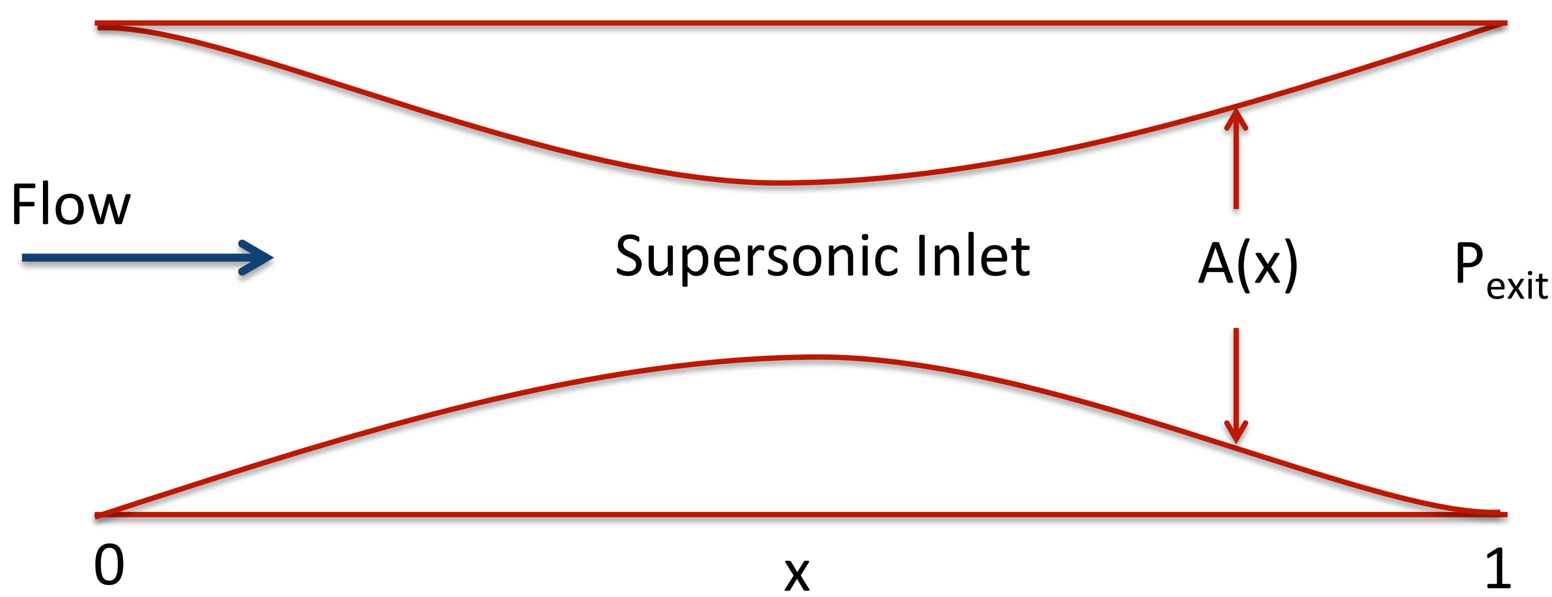
- Governing equation

$$\frac{\partial \boldsymbol{w}}{\partial t} + \frac{1}{A}\frac{\partial \boldsymbol{f} A}{\partial x} = \boldsymbol{q}$$

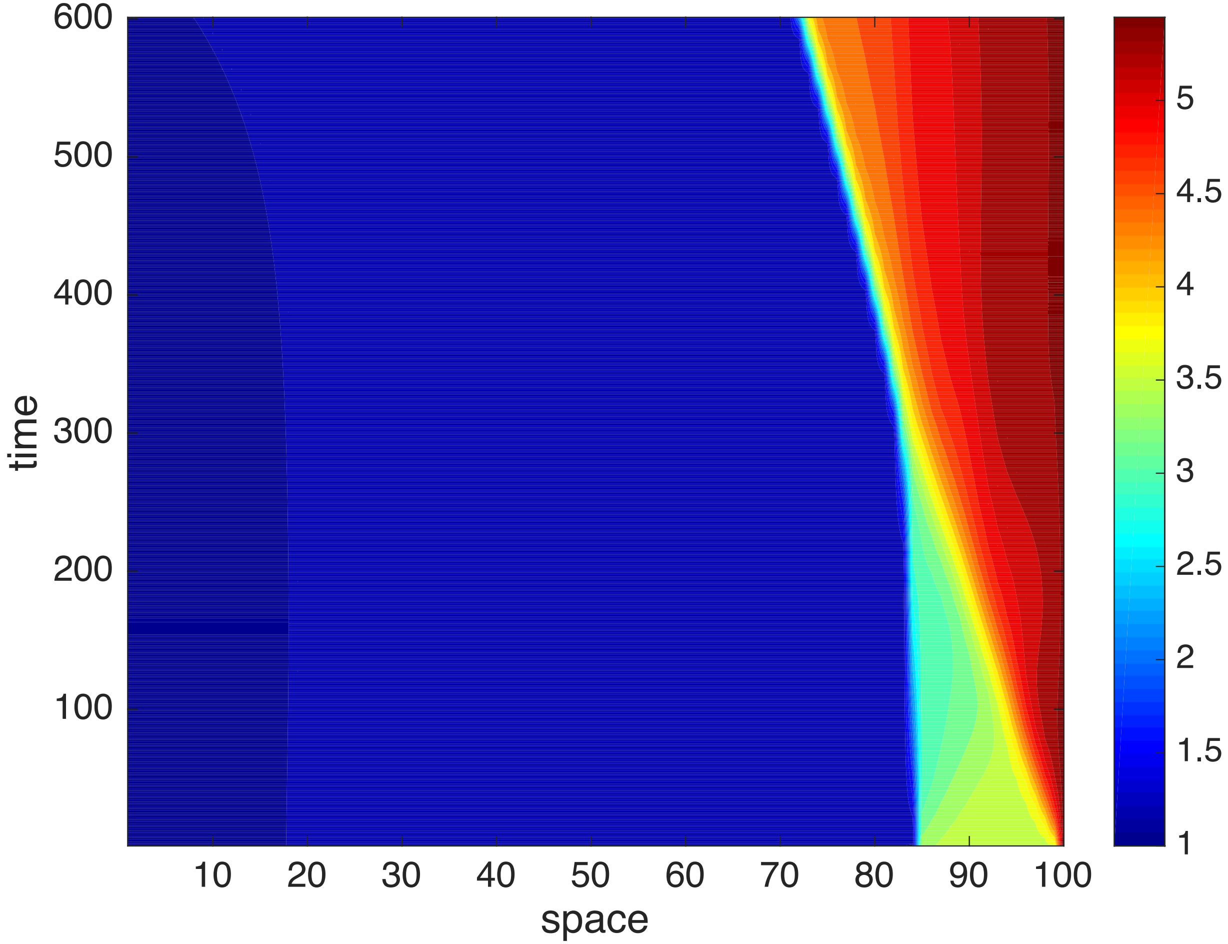
$$\boldsymbol{w} = \begin{bmatrix} \rho \\ \rho u \\ e \end{bmatrix} \qquad \boldsymbol{f} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (e+p)u \end{bmatrix} \qquad \boldsymbol{q} = \begin{bmatrix} 0 \\ \frac{p}{A}\frac{\partial A}{\partial x} \\ 0 \end{bmatrix}$$

- Spatial discretization: a finite volume method, $dx = 10^{-2}$
- Time integrator: implicit Row method,
- Parameter: exit pressure increase,

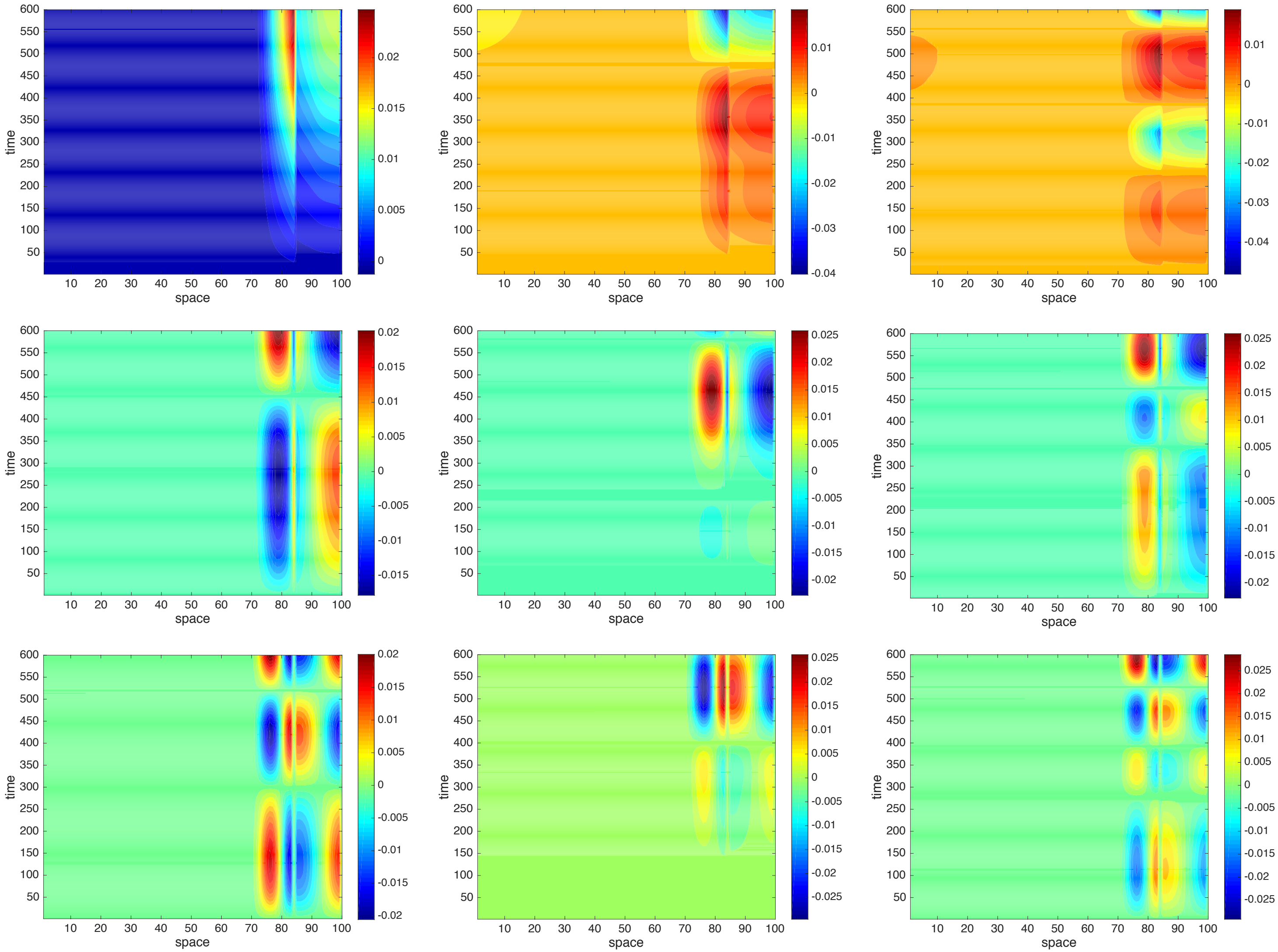
Moving Shock Problem



FOM solution

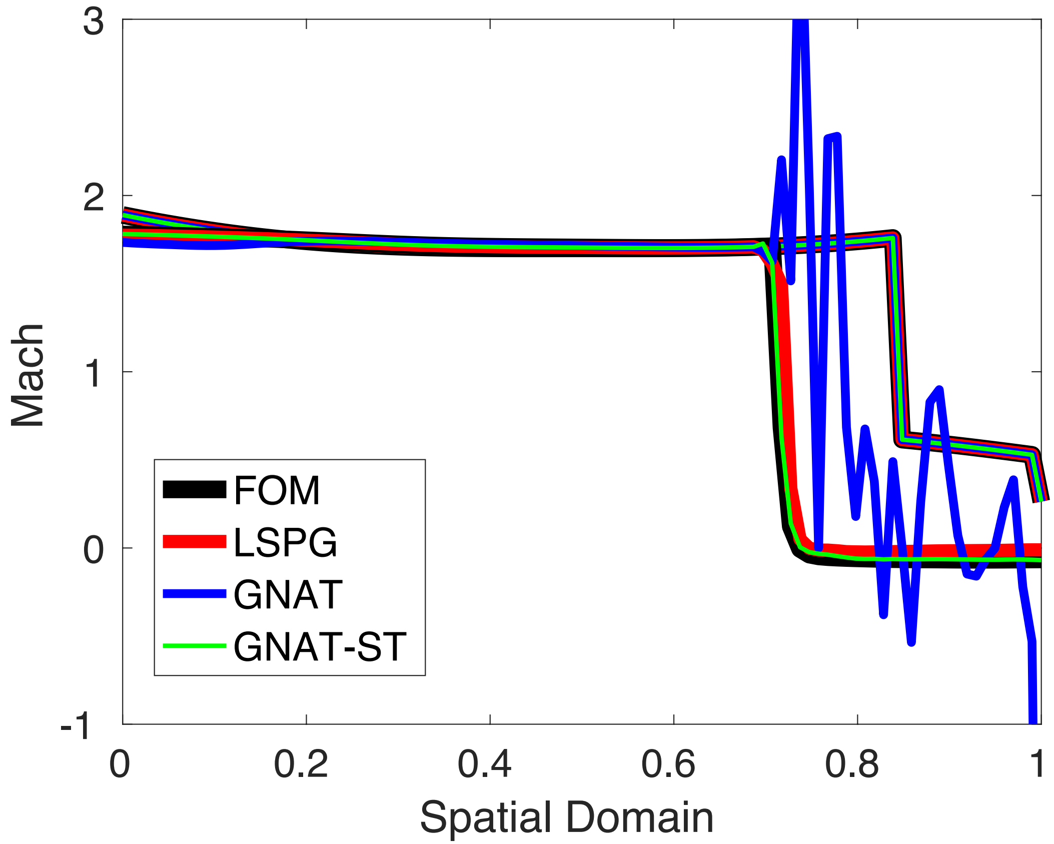


Spatiotemporal basis

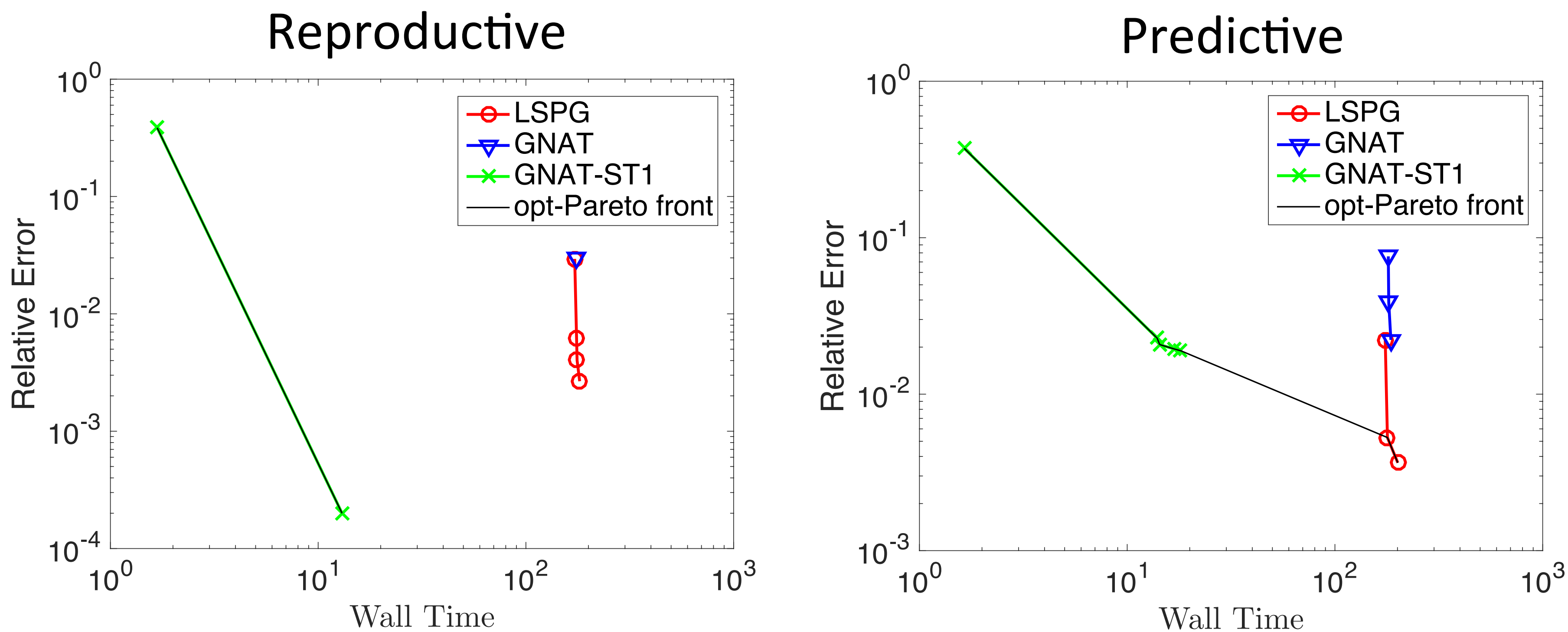


Mach History

- GNAT-ST is **8 times** faster than FOM (Full Order Model)
- GNAT fails at first time step



Optimal Pareto front



Conclusion

Accomplishment

+ Complexity is independence 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 HPC codes
- Apply the method in PDE-constrained optimization and UQ