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Space—time Least Squares Petrov-Galerkin Nonlinear Model Reduction

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Motivation

- Many applications require **long-time integration**, leading to **many time steps**
- Typical ROM apply **spatial projection**.
  - \+ Reduces spatial complexity
  - \- Does not reduce the temporal complexity: number of time steps remains large

Existing Work

- Explicit time integration [KRYSL]
  - \+ Can take larger stable time steps with ROMs,
  - \- Limited realizable speedup; not applicable to stiff
- Space–time finite–element full-order models [YANO, URBAN/PATERA]
  - \+ Error bounds grow linearly in time
  - \- Require a different full-order-model formulation; not always practical

Proposed Method

- **Main idea:** space—time projection to fully discrete, implicit nonlinear ODE models
- **Projection:** Least-squares Petrov–Galerkin projection to space–time discrete residual
- **Hyper-reduction:** Sample specific elements of the space–time discrete residual

Full-order Model

- **Ordinary Differential Equation (ODE)**

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

where $\boldsymbol{w} : [0,T] \to \mathbb{R}^{N_S}$ is the state, $\boldsymbol{w}_0 \in \mathbb{R}^{N_S}$ the initial condition, $\mathbf{f} : \mathbb{R}^{N_S} \times [0,T] \to \mathbb{R}^{N_S}$ is a nonlinear function, and $\boldsymbol{\mu} \in \mathbb{R}^{N_P}$ is a parameter vector.

- In linear multistep schemes, a residual at time step n is defined as

$$\boldsymbol{r}^{(n)}(\boldsymbol{w}) := \alpha_0 \boldsymbol{w} - \Delta t \beta_0 \mathbf{f}(\boldsymbol{w}, t^n) + \sum_{j=1}^{k} \alpha_j \boldsymbol{w}^{n-j} - \Delta t \sum_{j=1}^{k} \beta_j \mathbf{f}(\boldsymbol{w}^{n-j}, t^{n-j})$$

where Δt is the time step, the coefficients α_j and β_j define a specific linear multistep scheme.

Spatial Projection

- Solution approximation

$$\tilde{\boldsymbol{w}}(t^n) = \boldsymbol{w}_0 + \boldsymbol{V}\hat{\boldsymbol{w}}(t^n)$$

- $\boldsymbol{V} = [v_1 \;\; v_2 \;\; \dots \;\; v_{n_S}]$
- Solution subspace

$$\tilde{\boldsymbol{w}} \in \boldsymbol{w}_0 \otimes \mathbf{e}_T + \mathcal{S} \otimes \mathbb{R}^{N_t} \subseteq \mathbb{R}^{N_s} \otimes \mathbb{R}^{N_t}$$

- Spatial subspace
  - $\mathcal{S} := \mathrm{Ran}(\boldsymbol{V}) \subset \mathbb{R}^{N_s}$
  - $\dim(\mathcal{S}) = n_s$
- $\dim(\mathcal{S} \otimes \mathbb{R}^{N_t}) = n_s N_t$

Spatio-temporal Projection

- Solution approximation

$$\tilde{\boldsymbol{w}}(t^n) = \boldsymbol{w}_0 + \sum_{i=1}^{n_s} \sum_{j=1}^{n_t^i} \boldsymbol{v}_i u_{jn}^i \hat{w}_{ij}$$

- Solution subspace

$$\tilde{\boldsymbol{w}} \in \boldsymbol{w}_0 \otimes \mathbf{e}_T + \oplus_{i=1}^{n_s} \mathcal{S}_i \otimes \mathcal{T}_i \subseteq \mathbb{R}^{N_s} \otimes \mathbb{R}^{N_t}$$

- Spatial subspaces

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

- Temporal subspaces

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

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

Spatial LSPG

- Space discrete residual minimization problem at time step n

$$\hat{\boldsymbol{w}}^n = \arg \min_{\boldsymbol{y} \in \mathbb{R}^{n_s}} \|\mathbf{G}\boldsymbol{r}^{(n)}(\boldsymbol{w}_0 + \boldsymbol{V}\boldsymbol{y})\|_2^2$$

- LSPG: $\mathbf{G} = \mathbf{I}$
  GNAT: $\mathbf{G} = (\mathbf{Z}\boldsymbol{\Phi}_r)^{\dagger}\mathbf{Z}$

Spatio-temporal LSPG

- Space—time discrete residual minimization problem over the whole time

$$\hat{\boldsymbol{w}} = \arg\min_{\hat{\boldsymbol{y}}} \|\mathbf{G}\mathrm{vec}\left(\boldsymbol{r}(\bar{\boldsymbol{w}}_0 + \sum_{i=1}^{n_s} \sum_{j=1}^{\dim \mathcal{T}_i} \boldsymbol{v}_i \boldsymbol{u}_j^{i\,T} \hat{y}_{ij})\right)\|_2^2$$

- LSPG: $\mathbf{G} = \mathbf{I}$
  GNAT: $\mathbf{G} = (\overline{\boldsymbol{Z}\boldsymbol{\Phi}}_r)^{\dagger}\overline{\boldsymbol{Z}}$

Spatial Error Bound

- Backward Euler time integration

$$\|\boldsymbol{w}_\star^n - \boldsymbol{w}_{PG}^n\|_2 \leq 2\frac{\exp(t^n \kappa \epsilon^{-1}) - 1}{\kappa \Delta t} \max_{j \in \mathbb{N}(n)} \|\boldsymbol{r}^{(j)}(\tilde{\boldsymbol{w}}_{\mathrm{PG}}^j)\|_2$$

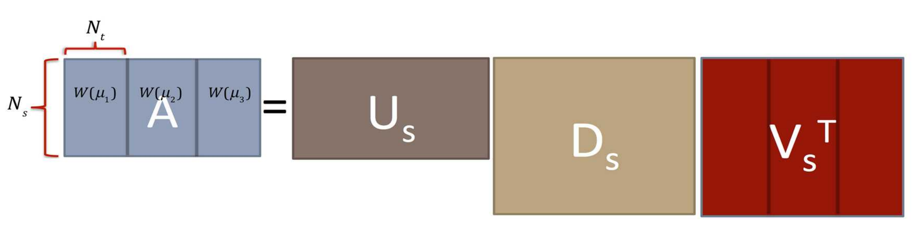
Spatio-temporal Error Bound

For backward Euler time integration

$$\|\boldsymbol{w}_\star^n - \boldsymbol{w}_{PG}^n\|_2 \leq \frac{\Delta t}{h_n}\|P_n(\boldsymbol{T}_{BE}^{-1} - \mathbb{P})\bar{\boldsymbol{f}}(\bar{\boldsymbol{w}}^{(0)} + \bar{\boldsymbol{w}}_{PG})\|_2$$

Subspace Generation

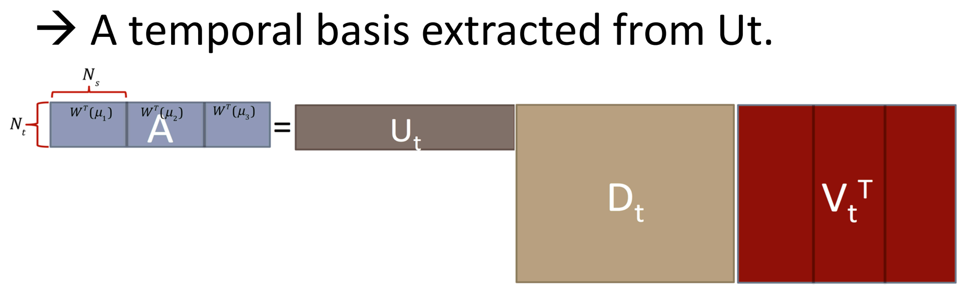
- Spatial Subspace



set $\mathbf{V} = [\mathbf{u}_S^1 \;\; \mathbf{u}_S^2 \;\; \dots \;\; \mathbf{u}_S^{n_S}]$

- Two ways of extracting temporal basis:

1. A diagonal matrix D_s pairs a column in Us with a column in Vs
   → three temporal modes extracted for each spatial mode from each column in Vs.
2. Temporal modes from Temporal SVD below:
   → A temporal basis extracted from Ut.



→ Equivalent to T-HOSVD [TUCKER]
→ More efficient way:
ST-HOSVD [VANNIEUWENHOVEN]

Snapshot Collection

- Train Set: $\mathcal{D}_{\mathrm{train}} := \{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_q\}$
- Snapshots: $\mathbf{W}(\boldsymbol{\mu}_i) = [\boldsymbol{w}^1(\boldsymbol{\mu}_i) \;\; \cdots \;\; \boldsymbol{w}^{N_t}(\boldsymbol{\mu}_i)]$
- Global Snapshots: $\mathbf{A} := [\mathbf{W}(\boldsymbol{\mu}_1) \;\; \dots \;\; \mathbf{W}(\boldsymbol{\mu}_q)]$

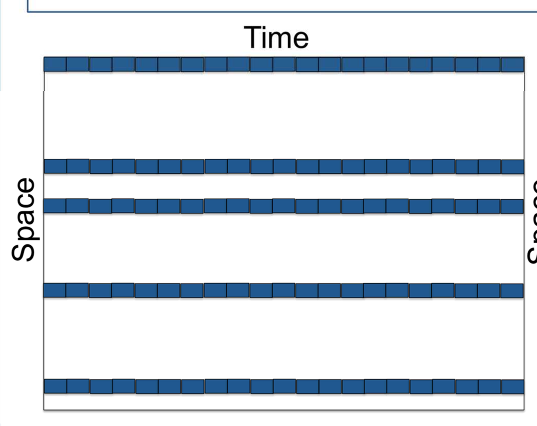


Figure 1. Spatial GNAT Z

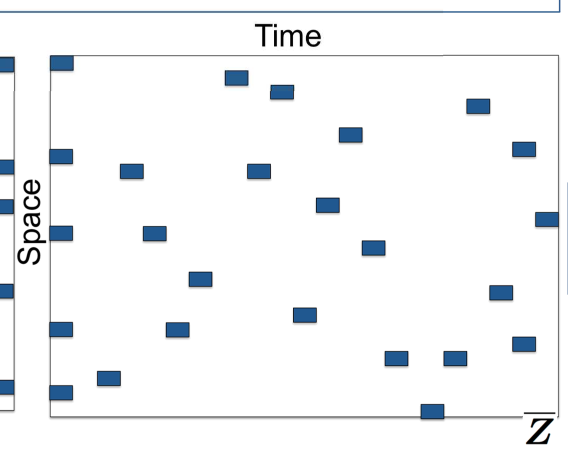


Figure 2. Spatio-temporal GNAT

Algorithm 1 Greedy algorithm for constructing sample-time set $\mathcal{T}$

Input: $\overline{\boldsymbol{\Phi}}_r$, target number of sample time n_{ti}
Output: sample-time set $\mathcal{T}$

$\mathcal{N} \leftarrow \{1, \dots, N_s\}$
$a_i \leftarrow \| \left[\overline{\phi}_{r(N_s(i-1),1)} \;\; \cdots \;\; \overline{\phi}_{r(N_s i,1)}\right] \|_2^2$ for $i = 1, \dots, N_t$
Find $k \in \{1, \dots, N_t\}$ such that $a_k \geq a_i, \forall i \in \{1, \dots, N_t\}$
$\mathcal{T} \leftarrow \{k\}$
for $j = 2, \dots, n_{ti}$ **do**
  for $\ell = 1, \dots, n_r$ **do**
    $\mathbf{R}^\ell \leftarrow \overline{\boldsymbol{\phi}}_r^\ell - \left[\overline{\boldsymbol{\phi}}_r^1 \;\; \cdots \;\; \overline{\boldsymbol{\phi}}_r^j\right]\alpha$, with $\alpha = \arg\min_{\gamma \in \mathbb{R}^j} \|\overline{\boldsymbol{Z}}\left[\overline{\boldsymbol{\phi}}_r^1 \;\; \cdots \;\; \overline{\boldsymbol{\phi}}_r^j\right]\gamma - \overline{\boldsymbol{Z}\boldsymbol{\phi}}_r^\ell\|_2$
  end for
  $q_m \leftarrow \sum_{\ell=1}^{n_r} |r_{(m,\ell)}|$ for $m = 1, \dots, N_t N_s$
  $a_i \leftarrow \| \left[q_{N_s(i-1)} \;\; \cdots \;\; q_{N_s i}\right] \|_2^2$ for $i = 1, \dots, N_t$
  Find $k \in \{1, \dots, N_t\}$ such that $a_k \geq a_i, \forall i \in \{1, \dots, N_t\}$
  $\mathcal{T} \leftarrow \mathcal{T} \cup \{k\}$
end for

Algorithm 2 Greedy algorithm for constructing sample-node set $\mathcal{N}$

Input: $\overline{\boldsymbol{\Phi}}_r$, $\mathcal{T}$, target number of sample nodes n_{si}
Output: sample-node set $\mathcal{N}$.

$\mathcal{I}_a \leftarrow \{1, \dots, N_s N_t\}$
Find $k \in \mathcal{I}_a$ such that $|\overline{\phi}_{r(k,1)}| \geq |\overline{\phi}_{r(i,1)}|, \forall i \in \mathcal{I}_a$
$\mathcal{N} \leftarrow \mathcal{I}_a \cap [k]_{N_s}$ where $[k]_{N_s}$ is a congruence mod N_s.
$\mathcal{I}_i \leftarrow [k]_{N_s}$
for $j = 2, \dots, n_{si}$ **do**
  for $\ell = 1, \dots, n_r$ **do**
    $\mathbf{R}^\ell \leftarrow \overline{\boldsymbol{\phi}}_r^\ell - \left[\overline{\boldsymbol{\phi}}_r^1 \;\; \cdots \;\; \overline{\boldsymbol{\phi}}_r^j\right]\alpha$, with $\alpha = \arg\min_{\gamma \in \mathbb{R}^j} \|\overline{\boldsymbol{Z}}\left[\overline{\boldsymbol{\phi}}_r^1 \;\; \cdots \;\; \overline{\boldsymbol{\phi}}_r^j\right]\gamma - \overline{\boldsymbol{Z}\boldsymbol{\phi}}_r^\ell\|_2$
  end for
  $q_m \leftarrow \sum_{\ell=1}^{n_r} |r_{(m,\ell)}|, \forall m \in \mathcal{I}_a$
  Find $k \in \mathcal{I}_a - \mathcal{I}_i$ such that $q_k \geq q_i, \forall i \in \mathcal{I}_a - \mathcal{I}_i$
  $\mathcal{N} \leftarrow \mathcal{N} \cup (\mathcal{I}_a \cap [k]_{N_s})$, $\mathcal{I}_i \leftarrow \mathcal{I}_i \cup [k]_{N_s}$
end for

Numerical Experiments

1D Burgers' equation

- Governing Equation

$$\frac{\partial w(x,t)}{\partial t} + \frac{\partial f(w(x,t))}{\partial x} = g(x) \qquad w(0,t) = \mu \qquad w(x,0) = q(x)$$

- Spatial discretization : a finite volume method
- Time integrator : the Backward Euler method
- Solution History and Pareto Fronts (10x faster)

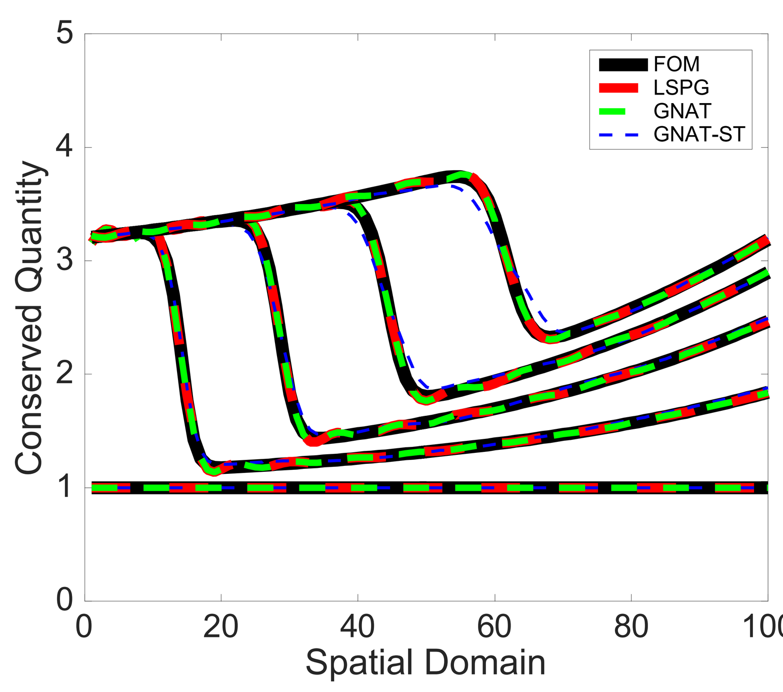


Figure 3. Solution History

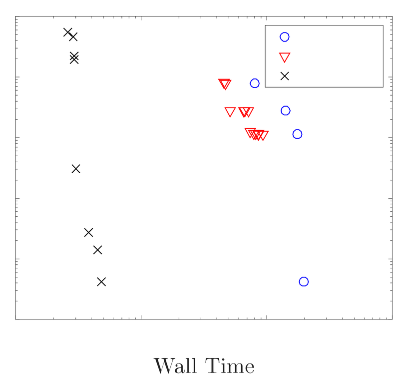


Figure 4. Reproductive

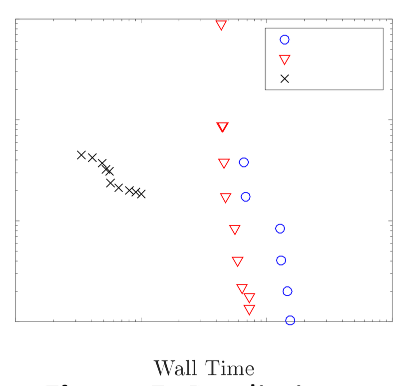


Figure 5. Predictive

Conclusion

- Have introduced a reduced order model for nonlinear dynamic system whose complexity is independent of both space and time
- The construction was purely algebraic
- The formulation does not depend on space—time FEM
- Any implicit time integration can be used to build a ROM
- Showed very promising results
- Need to seek a way of improving accuracy for reproductive case
- Next step: try a bigger problem. Implement in SPARC and Albany

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