ACCELERATING THE ANALYST WORKFLOW: ADAPTIVE HYBRID MODELS VIA DOMAIN DECOMPOSITION (AHEAD)

ESRF LDRD PROJECT, YEAR 2 OUT OF 3

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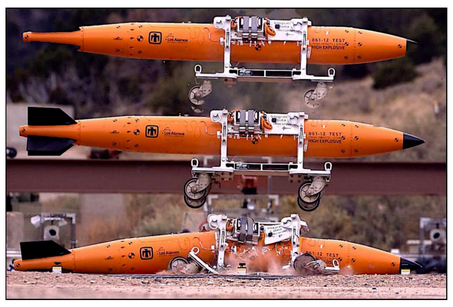
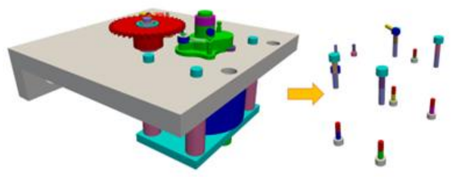
Motivation

- Analyses involving **high-fidelity models (HFMs)** and codes can be **prohibitive** due to:
  (i) **mesh generation** challenges, and
  (ii) **long runtime** requirements
- Data-driven **reduced order models (ROMs)** promise to mitigate challenge (ii) but:
  - ➢ Suffer from **lack** of **stability/accuracy** for predictions
  - ➢ **Cannot** be **easily refined** to achieve a specified level of accuracy like conventional discretizations

Goal of AHEAD: mitigate above challenges through **hybrid (ROM + high-fidelity) models** based on **optimal domain decomposition (DD)** and the **Schwarz alternating method (SAM)**

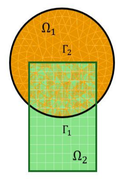


B61-12 guided drop test. SAND 2018-13067M,



Ratcheting mechanism with multiple threaded fasteners. From Parish *et al.*, 2024.

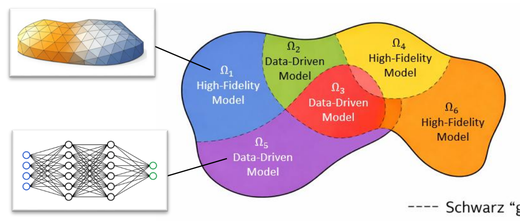
Technical Approach



Basic Schwarz alternating method (SAM) scheme for coupling [1-2]

- Decompose $\Omega = \Omega_1 \cup \Omega_2$
- Solve PDE in Ω_2 w/ boundary conditions (BCs) on Γ_2 from just-obtained Ω_1 solution.
- Solve PDE in Ω_1 w/ BCs on Γ_1 from just-obtained Ω_2 solution.
- Iterate until convergence

SAM enables the **seamless plug-and-play coupling** of disparate **meshes**, **solvers**, **time-steppers** and **models** (ROM+HFM) [1-7].

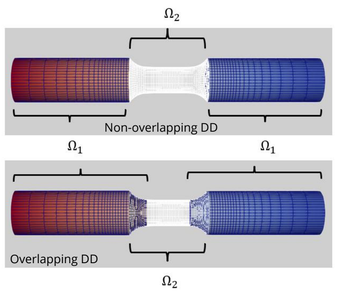


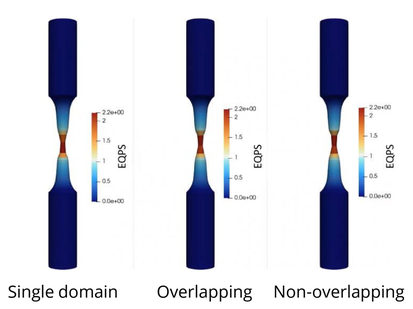
New R&D under AHEAD

- **Non-overlapping SAM** for better flexibility [3,6-7]
- SAM for the rigorous coupling of **non-intrusive Operator Inference (OpInf) ROMs** [5-6]
- **Online mesh/model switching** and **refinement** based on rational, automated criteria

High-Fidelity Model (HFM) Coupling

Tension Specimen

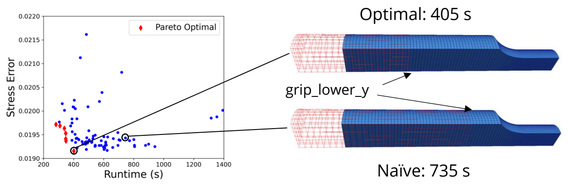




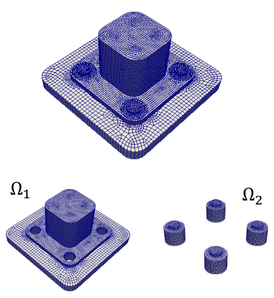
Non-overlapping and overlapping SAM in **SIERRA/SM** can **correctly predict necking** in cylindrical tensile specimen geometry with **errors < 0.1%.**

Risk: manual SAM DD **tuning** is often **expert-driven**, **trial-and-error**, **costly** and **tedious**.

Mitigation: **multi-objective optimization** of DD using GPTune



Bolted Joint



Overlapping DD

	CPU times (64 procs)	Avg # SAM iterations	Max # SAM iterations
Single Domain	46m 45s	–	–
Schwarz	15m 43s	3.0	3
Single Domain (finer mesh)	4h 10m 3s	–	–
Schwarz (finer mesh of bolts)	1hr 43m 12s	3.0	3

Despite its iterative nature, SAM can be **faster** than comparable single domain run!

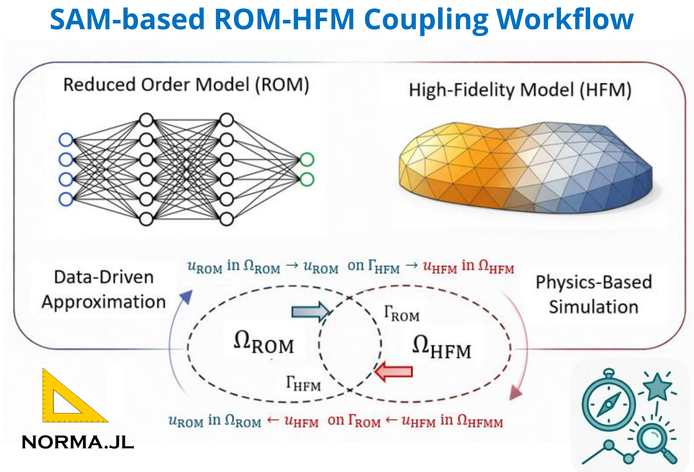
Benefit: SAM **significantly simplifies meshing** and **transforms** hard multiscale problem in Ω into **easier monoscale problems** in Ω_i

Reduced Order Model (ROM) Coupling

Non-intrusive OpInf ROMs

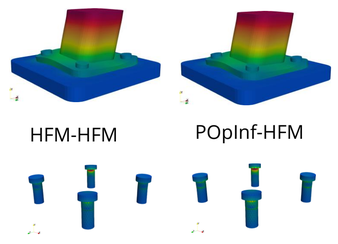
- Define **ROM model form** in each subdomain: $\dot{\hat{\boldsymbol{q}}} + \hat{\boldsymbol{F}}(\hat{\boldsymbol{q}}) = \boldsymbol{0}$
- **ROM model forms:**
  - ➢ Polynomial (P): $\hat{\boldsymbol{F}}(\hat{\boldsymbol{q}}) = \hat{\boldsymbol{A}}\hat{\boldsymbol{q}} + \hat{\boldsymbol{H}}(\hat{\boldsymbol{q}}\otimes\hat{\boldsymbol{q}}) + \hat{\boldsymbol{G}}(\hat{\boldsymbol{q}}\otimes\hat{\boldsymbol{q}}\otimes\hat{\boldsymbol{q}})$ [5-6]
  - ➢ Neural Network (NN): $\hat{\boldsymbol{F}}(\hat{\boldsymbol{q}}) = \boldsymbol{K}(\hat{\boldsymbol{q}};\boldsymbol{w})\hat{\boldsymbol{q}} \rightarrow$ enables **structure preservation (SP)** [8]
- **Infer** operators from HFM data by solving **optimization problem**

SAM-based ROM-HFM Coupling Workflow

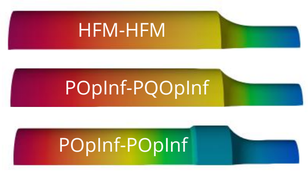


Bolted Joint

All hybrid models **correctly predict** the location of maximum von Mises stress (**failure**) even in **predictive regime**



Tension Specimen

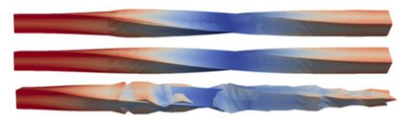


(competing method, Farcas *et al.*, 2024 gives incorrect solution)

POpInf-POpInf TET10-HEX8 couplings achieve impressive **106× speedup** while maintaining ***O*(0.1%) errors** in **predictive regime**

Torsion

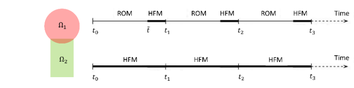
Couplings involving **Lagrangian structure-preserving NN-OpInf ROMs** can maintain **stability** and **robustness** in **predicting future state**



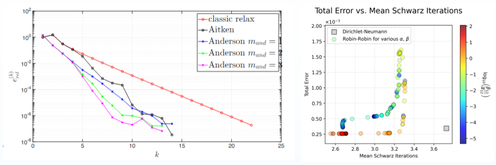
Top: HFM-HFM
Middle: HFM-NNOpInf with SP
Bottom: HFM-POpInf

Ongoing & Future Work

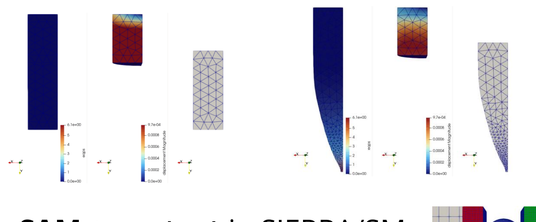
- **ROM implementation** in SIERRA/SM
- **Online ROM-HFM switching**



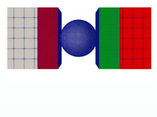
- **SAM acceleration strategies**: Aitken and Anderson acceleration [7], inexact Schwarz, Robin-Robin non-overlapping Schwarz [6]



- **SAM + in-core remeshing** in SIERRA/SM



- **SAM + contact** in SIERRA/SM
- **SAM + Craig-Bampton Reduction (super-elements)** in SIERRA/SM and comparison to SAM + OpInf



Strategic Alignment

- Improve analyst output by **reducing meshing time** by at least an order of magnitude
- Provide **credible mechanism to integrate data-driven ROMs** into mod/sim workflows while **maintaining desired level of accuracy** and **achieving speedups**
- Enable **heterogeneous multi-scale** and **multi-physics** simulations involving different types of models with different fidelities
- Develop a **rational way** to determine **when** and **where** to use more refined model **on-the-fly,** providing analysists with **smart, hands-off workflow** to **inform design decisions**

Team

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Outcomes

- **Journal articles**: 2 published, 3 submitted; **Proceedings papers:** 2 published
- **12 invited conference presentations/university seminars**, including **1 invited plenary** presentation at CILAMCE 2025; 5 internal presentations
- **4** open-source **code releases**
- **1 post doc converted** to staff
- Obtained **funding** for synergistic project under DOE+DOW **Joint Munitions Program**

References

[1] A. Mota, I. Tezaur, C. Alleman. "The Schwarz alternating method in solid mechanics", *Comput. Meth. Appl. Mech. Engng.* 319 19-51, 2017.
[2] A. Mota, I. Tezaur, G. Phlipot. "The Schwarz alternating method for dynamic solid mechanics", *Int. J. Numer. Meth. Engng.* 123 (21) 5036-5071, 2022.
[3] A. Mota, D. Koliesnikova, I. Tezaur, J. Hoy. "A Fundamentally New Coupled Approach to Contact Mechanics via the Dirichlet-Neumann Schwarz Alternating Method", *Int. J. Numer. Meth. Engng.*, 126(9) e70039, 2025.
[4] C. Wentland, F. Rizzi, J. Barnett, I. Tezaur. "The role of interface boundary conditions and sampling strategies for Schwarz-based coupling of projection-based reduced order models", *J. Comput. Appl. Math.,* 465 116584, 2025.
[5] I. Tezaur, E. Parish, A. Gruber, I. Moore, C. Wentland, A. Mota. "Hybrid coupling with OpInf and the SAM", submitted to *IJNME*.
[6] C. Rodriguez, I. Tezaur, A. Mota, A. Gruber, E. Parish, C. Wentland. "Transmission Conditions for the Non-Overlapping Schwarz Coupling of Full Order and Operator Inference Models", CSRI Summer Proceedings 2025, Sandia National Laboratories, Albuquerque, NM & Livermore, CA (2025).
[7] G. Sambataro, I. Tezaur. "On the role of relaxation and acceleration in the non-overlapping SAM for coupling", submitted to *JCAM*.
[8] E. Parish, A. Gruber, P. Blonigan, I. Tezaur. "NN-OpInf: an OpInf approach using structure-preserving composable NNs", submitted to *JCP*.

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