College of Science
CENTER FOR MATHEMATICS AND ARTIFICIAL INTELLIGENCE
George Mason University

Digital Twins: A PDE–Constrained Optimization Perspective

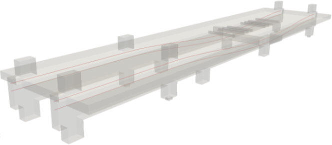
Harbir Antil

Center for Mathematics and Artificial Intelligence (CMAI) and
Department of Mathematical Sciences
George Mason University
hantil@gmu.edu

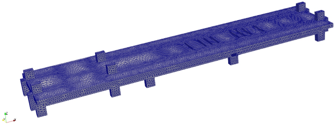
November 19-25, 2025

The Mathematics of Scientific Machine Learning and Digital Twins
International School of Mathematics "G. Stampacchia", Erice, Italy

Concerto Bridge (TU Braunschweig)



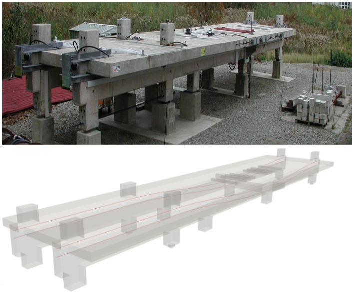
Physical asset



Digital Model

- **Classical model:** Under a given load configuration, numerical results matches the measurements.

Concerto Bridge (TU Braunschweig)



Physical asset

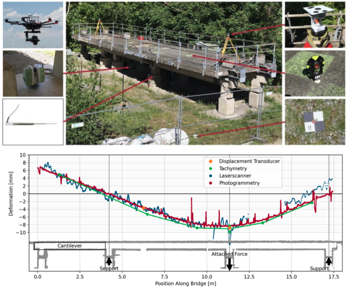
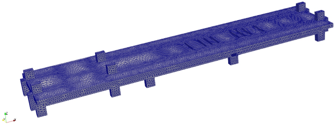


Figure 17. Measured deformation along the centre profile of the bridge between Epoch 3 and 4 (loading).

Sensor measurements



Digital Model

- **Classical model:** Under a given load configuration, numerical results matches the measurements.
- **Towards Digital Twin:** From these measurements, can we identify weak spots?
- **Key components:**

  physical asset → data (e.g. sensors) → digital model (family) → a feedback loop
- These are **optimization problems with constraints** that must account for **uncertainty**.

References: NASEM [Willcox et al (2023)]; [A. (2024)] arXiv:2402.10326.

Recent Examples of Bridge Failures

Minneapolis (2007)

Genoa (2018)

Dresden (2024)

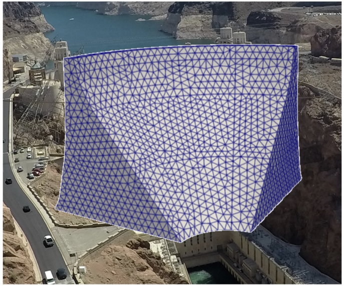
Reality Meets Digital Twins

Hoover dam (USA)

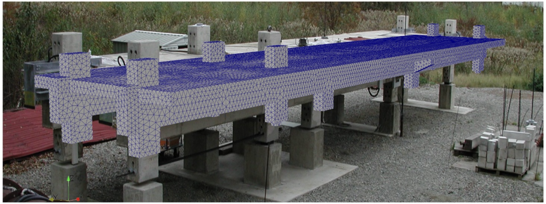
Concerto bridge (TUBS)

Vilinius bridge (Lithuania)

Reality Meets Digital Twins



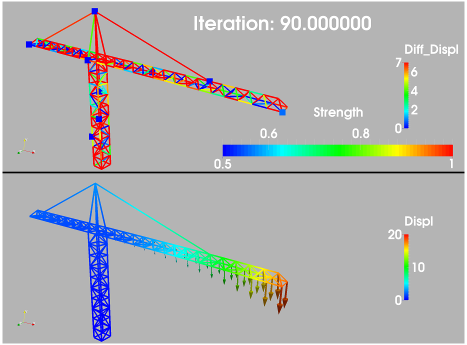
Hoover dam (USA)



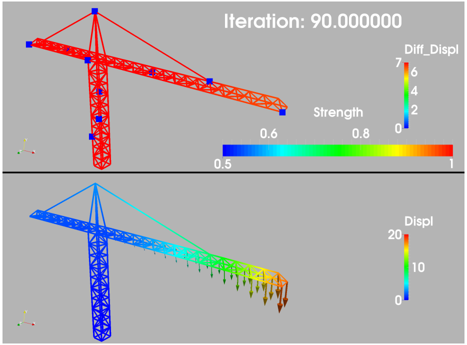
Concerto bridge (TUBS)

Vilinius bridge (Lithuania)

Incorrect Scalar Products [Airaudo, A., Löhner, Wüchner (2024)]



(a) Incorrect Scalar Product



(b) Correct Scalar Product

- **Non structure-preserving** discretizations can lead to incorrect results.
- **Existence of solution** to infinte diam. optimization problems – Identify appropriate function spaces. [A., Kouri, Ridzal, Robinson, Salloum (2024)]
- **Large scale (infinite diam.)** optimization – Design algorithms which can handle inexactness. [A., Kouri, Ridzal (2024)], [A., Lentz (2025)] and [A., Kouri, Baraldi (2025)]
- **Uncertainty** in PDECO and Digital Twins

Inexact Algorithms to Solve PDECO Problems

- [A., Kouri, Ridzal, 2023]: *ALESQP: An augmented Lagrangian equality-constrained SQP method for optimization with general constraints.* SIAM J. of Optimization. 2023

$$\min_{u,z} f(u,z) \quad \text{subject to} \quad c(u,z)=0, \quad T_1 z \in C_1, \quad T_2 u \in C_2$$

- [A., Lentz, 2025]: *A Smoothed Proximal Trust-Region Algorithm for Nonconvex Optimization with L^p-regularization, $p \in (0,1)$.* Submitted, 2025

$$\min_{u,z} f(u,z) + g(z) \quad \text{subject to} \quad c(u,z)=0, \quad T_1 z \in C_1$$

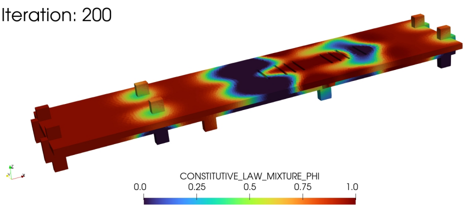
where f is smooth but nonconvex and g is nonsmooth and nonconvex.

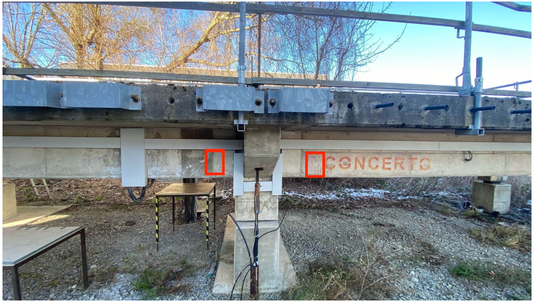
- [A., Baraldi, Kouri, 2025]: *Memory-Efficient Nonsmooth Dynamic Optimization using Adaptive Randomized Compression.* Submitted 2025.

$$\min_{u_n \in \mathbb{R}^M, z_n \in \mathbb{R}^m} \sum_{n=1}^{N} f_n(u_{n-1}, u_n, z_n) + \sum_{n=1}^{N} \phi_n(z_n)$$

where $u_n \in \mathbb{R}^M$ solves: $\quad c_n(u_{n-1}, u_n, z_n) = 0, \quad n = 1, \ldots, N\,.$

Crack Identification





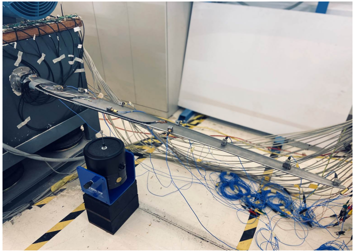
Thermal Effects?

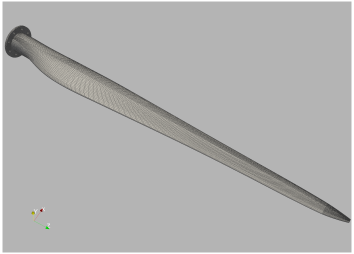
- The objects are subjected to sun, shade, snow, etc. The **thermal loading effect** can be higher than standard loading.
- Design standards in “American Association of State Highway and Transportation Officials (AASHTO) LRFD” focus on temperature distribution in vertical direction, which maybe inadequate and has been found untrue.
- Additionally, pre-specification of thermal loads are not real-time.

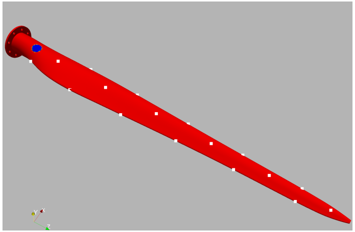
Ansari, Löhner, Wüchner, A., Warnakulasuriya, Antonau, Airaudo. Adjoint-Based Recovery of Thermal Fields From Displacement or Strain Measurements CMAME (2025).

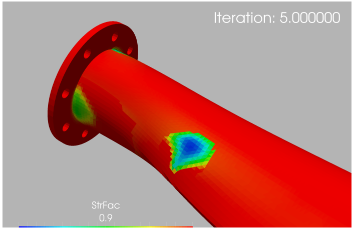
Concerto bridge (TUBS)

Wind Turbine Blade (Geometry Provided by SIEMENS)







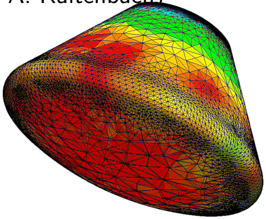


Digital Twins in Space: Designing Heat Shield

"Resurgence in demand for reusable thermal protective systems
is driving renewed research and development" (Caldwell et al., 2024)

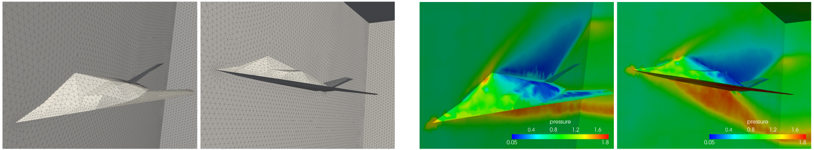
- ▶ **Sensors measure** remaining material distribution d_r and external temperature u_{ext}.
- ▶ Where to distribute replacement material optimally while ensuring that you can withstand u_{ext}.

- **Designing heat shield** (with K. Kirk and A. Kaltenbach)

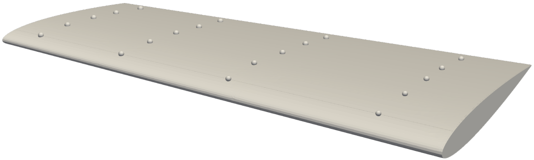


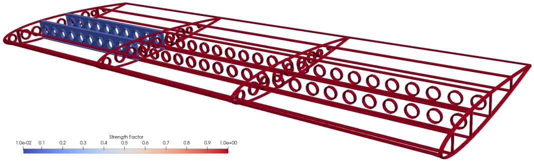
Motivated by: [G. Buttazzo (1988)]
[A., Kaltenbach, Kirk] (SIMA), [A., Kaltenbach, Kirk] (SICON), [A., Bartels, Kaltenbach, Khandelwal] (MathComp, 2025)

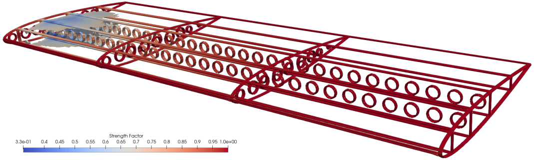
- **F117 in space** (with R. Löhner)

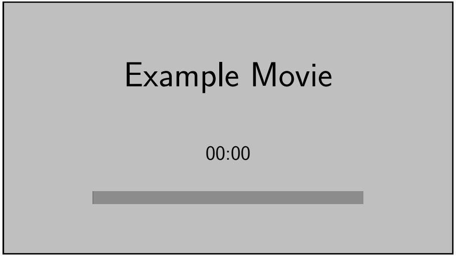


Dynamic Setting: Airplane Wing



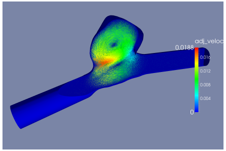


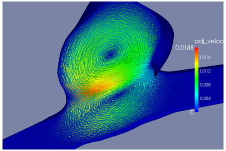




Medical Digital Twins

- **Examples of DT in healthcare**:
  - A **hospital system:** patients, providers, and operational performance.
  - A **person or organ** to simulate health conditions and treatment effects.
- **Examples of use cases:**
  - Real-time monitoring and analysis, improved telehealth.
  - Clinical trials and personalized medicine.
  - Optimization of hospital workflows by tracking patient and equipment movements.
  - DT population and enhancing clinical trial diversity
- Our work (with J. Cebral (Bioengineering) and R. Löhner (Physics)) is on aneurysms. **[A., Löhner, Cebral, Mut (2024)]**



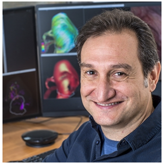


- **Reference:** "Digital twins in medicine" R. Laubenbacher, B. Mehrad, I. Shmulevich & N. Trayanova. Nature Computational Science volume 4, pages 184–191 (2024)

Digital Twins Lab

Harbir Antil (CMAI, Math)

Rainald Löhner (CFD, Physics)



Juan Cebral (Bioengineering)

Facundo Airaudo (CFD, Physics)

Roland Wüchner (TUM)

Talhah Ansari (TUM)

Suneth Warnakulasuriya (TUM)

Ihar Antonau (TU Braunschweig)

Denis Ridzal (Sandia Labs)

Drew Kouri (Sandia Labs)

In collaboration with:

- Technical University Munich
- Sandia National Labs and SIEMENS

Conclusions So Far

- **Optimization based DT framework** to identify weakness in structures is introduced.
- **Structure preserving** discretization and algorithms are needed to solve these problems.
- The computational experiments have been validated against **real experiments**.

Math (selected):

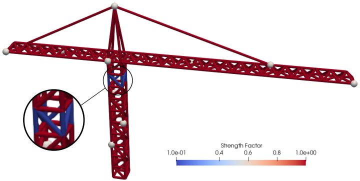
- H. Antil, S. Carney, H. Díaz and J. Royset. *Rockafellian Relaxation for PDE Constrained Optimization with Distributional Ambiguity.* arXiv:2405.00176v1 (2024).
- H. Antil, D.P. Kouri, D. Ridzal. ALESQP: An Augmented Lagrangian Equality-constrained SQP Method for Optimization with General Constraints. SIOPT (2023).
- H. Antil, D.P. Kouri, D. Ridzal, D.B. Robinson, and M. Salloum. *Uniform flow in axisymmetric devices through permeability optimization.* OPTE (2023).
- H. Antil, S. Dolgov and A. Onwunta. *TTRISK: Tensor Train Decomposition Algorithm for Risk Averse Optimization.* NLAA (2022).
- H. Antil, Drew Kouri, Martin Lacasse, and Denis Ridzal. *Frontiers in PDE-constrained Optimization.* The IMA Volume, 2018.

Digital Twins (selected):

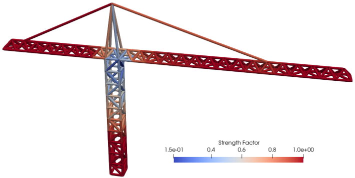
- T.S.A. Ansari, R. Löhner, R. Wüchner, H. Antil, K-U. Bletzinger, S. Warnakulasuriya, I. Antonau, and F. Airaudo. *Adjoint-Based Recovery of Thermal Fields From Displacement or Strain Measurements.* CMAME, 2025.
- F. Airaudo, H. Antil, R. Löhner. *Conditional Value at Risk to Identify Weaknesses in Structural Digital Twins.* FINEL, 2025.
- R. Löhner, H. Antil, S. Schoeps. *On Techniques for Barely Coupled Multiphysics.* AIAA 2025-0576 (2025). DOI: 10.2514/6.2025-0576.
- R. Loehner, F. Airaudo, H. Antil, R. Wuechner, S. Warnakulasuriya, I. Antonau and T. Ansari. *High-Fidelity Digital Twins: Zooming in on Weakness in Structures.* AIAA 2025-0286 (2025). DOI: 10.2514/6.2025-0286.
- I. Antonau, S. Warnakulasuriya, R. Wuechner, R. Loehner, F. Airaudo, H. Antil, and T. Ansari. *Comparison of the First Order Algorithms to Solve System Identification Problems of High-Fidelity Digital Twins.* AIAA 2025-0285 (2025). DOI: 10.2514/6.2025-0285.
- R. Löhner, F. Airaudo, H. Antil, R. Wuechner, F. Meister, S. Warnakulasuriya. *High-Fidelity Digital Twins: Detecting and Localizing Weaknesses in Structures.* IJNME, 2024.
- R. Löhner, H. Antil, J.R. Cebral, and F. Mut *Adjoint-Based Estimation of Sensitivity of Clinical Measures to Boundary Conditions for Arteries.* Journal of Computational Physics, 2024.
- F.N. Airaudo, R. Löhner, R. Wüchner, and H. Antil. *Adjoint-based Determination of Weaknesses in Structures.* CMAME, 2023.

What's next: Can the framework account for **uncertainty**?
TT decomposition, Risk-measures, Rockafellian relaxation.

Digital Twins and Curse of Dimensionality



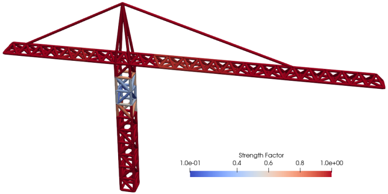
(a) Target strength factor



(b) $\mathbb{E}(X)$

- $\mathbb{E}[J(u, z; \xi)]$ does not account for rare but critical events. [Kouri, Surowiec (2016)], [Airaudo, A., Löhner, Rakhimov (2024)]
- High-dimensional integrals $\mathbb{E}[f] = \int_{\Xi} f(\xi)\rho(\xi)d\mu(\xi)$.
- How to quantify uncertainty level? CVaR_β?
- **Risk measures** are non-smooth

$$\text{CVaR}_\beta(J) := \inf_{t\in\mathbb{R}} \left\{ t + (1-\beta)^{-1}\mathbb{E}[(J-t)_+] \right\}$$



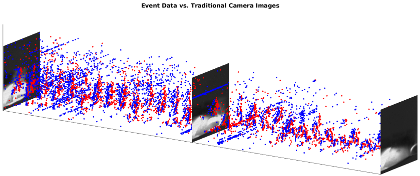
(c) $\text{CVaR}_{0.8}(X)$

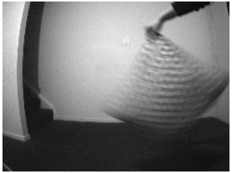
Tensor train decomposition: [A., Dolgov, Onwunta] (2022, 2024, 2025).

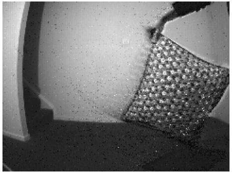
Question: What if we don't know the underlying distribution / corrupted? [A., Carney, Díaz, Royset (2024)]

Neuromorphic Imaging

- Some challenges with imaging technology
  - Many cameras are subject to motion blur.
  - Space-based cameras require significant power and storage, which is limited in space.
  - Tracking satellites or astronomical objects require working in high contrast environment.
- Optimization based models and algorithms have been developed for *neuromorphic cameras* [A., Sayre] Inverse Problems, 2023, 2024







- Research could have direct impact on our day-to-day life.

Real-time Latent Frame Generation with Falcon Neuro Data

- Feedback from the reconstruction can adjust camera position on ISS.

ISS (Source: USAFA SPARC)

Event Data

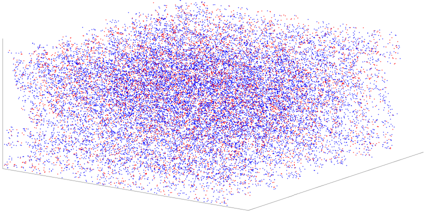
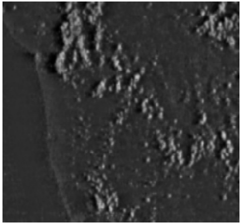


Image Reconstruction (Left: Antil, Sayre; Right: McHarg 2020)



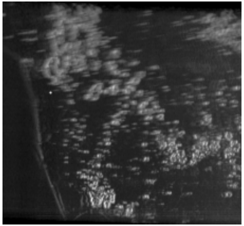


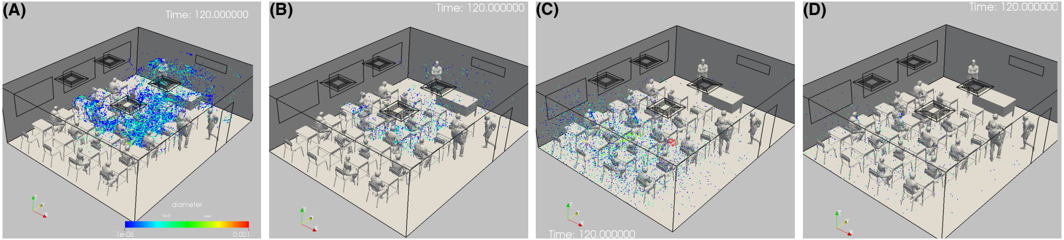
Image reconstruction is carried out by solving the optimization problem (per pixel) **[Antil, Sayre 2024]**:

$$\boldsymbol{v}_{xy} = \underset{\boldsymbol{v}_{xy}}{\operatorname{argmin}} \frac{1}{2}\|\boldsymbol{A}\boldsymbol{v}_{xy} - \boldsymbol{E}_{xy}\|_2^2 + \frac{\lambda}{2}\|\boldsymbol{v}_{xy}\|_2^2.$$

Dynamic Reconstruction [A., Blauvelt, Sayre, 2025]

Hospital Room

Airflow Simulations



- Navier Stokes (airflow) + ODEs (particles)
- Research has appeared in the **NY Times**, **NBC Today**, and multiple peer reviewed articles.
- We have worked with **DOJ**, in particular, Chief justices of MD, NYSD, NYED.
- Several **mitigation strategies** have been considered, from basic (such as wearing masks, proper ventilation) to more advanced (such as UV light).

Train Station

[A., Löhner: 2020, 2021, 2023]

From PDEs to Graph Diffusion Models

Motivation: When the domain of a Digital Twin is represented by a network (e.g., corridors), steady diffusion processes can be modeled by weighted graphs.

- Discrete analogue of $-\nabla\cdot(k\nabla u) = 0$ on a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$.
- Edge conductance: $c_e = k_e/L_e$; flux law $q_e = -c_e(u_{h(e)} - u_{t(e)})$.
- At node $v \in \mathcal{V}$, the nodal flux balance (inflow minus outflow) is

$$\Phi_v \;:=\; \sum_{e\in\mathcal{E}:\, h(e)=v} q_e \;-\; \sum_{e\in\mathcal{E}:\, t(e)=v} q_e, \qquad \sum_{v\in\mathcal{V}} \Phi_v = 0.$$

  Interior nodes enforce conservation: $\Phi_v = 0$ for all $v \notin \mathcal{V}_{\text{in}} \cup \mathcal{V}_{\text{out}}$.

Boundary control: Boundary potentials g act as control variables driving the interior state (u, q, Φ).

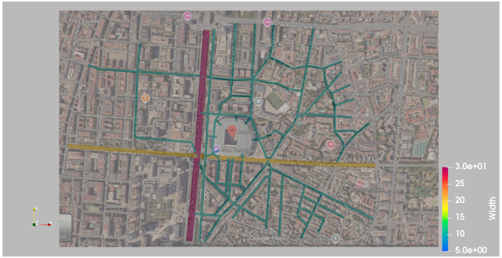
$$(u, q, \Phi) = (u_0, q_0, \Phi_0) + (U, Q, P)\, g.$$

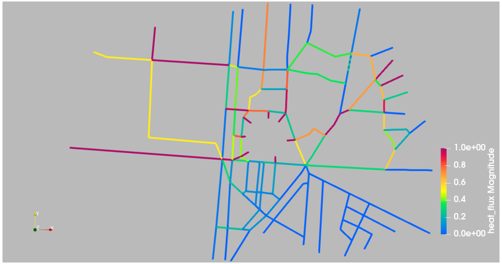
Optimization problem:

$$\min_g \; c^\top g \quad \text{s.t. } A_{\text{edge}} g \le b_{\text{edge}},\; A_{\text{cap}} g \le b_{\text{cap}},\; g_{\min} \le g \le g_{\max}.$$

$\Rightarrow$ A finite-dimensional *Linear Program (LP)* with physical constraints (sign, flux caps, box bounds).

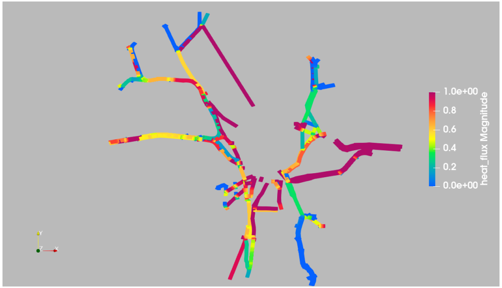
Real-World Demonstrations: Single Component

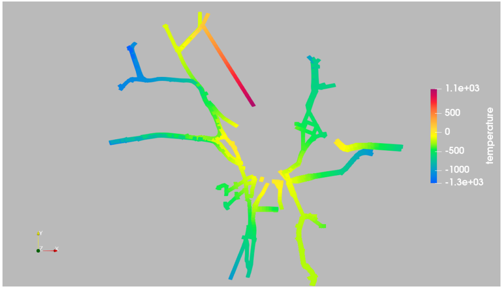




- Potential ("temperature") encodes a driving field – pressure, comfort, or urgency – that induces flux along the network.
- Flux gives the observable flow of people or material. Linked by $q_e = -c_e(u_{h(e)} - u_{t(e)})$

Real-World Demonstrations: Multi-Component





- LP enforces sign and flux-cap constraints on each boundary edge.
- Fluxes conserve to within 10^{-13} (double-precision tolerance).
- Extends naturally to other diffusive processes (thermal, chemical, crowd flow).

Takeaway: Diffusion on graphs provides a discrete, LP-solvable surrogate for PDE-constrained Digital Twins.

[A., Löhner, Pérez (2025)]

Optimal Cloaking Problem

$$\min_{z\in L^2(\Omega)} \frac{1}{2}\left(\|E-E_d\|^2_{L^2(0,T;L^2(\Omega))} + \|B-B_d\|^2_{L^2(0,T;L^2(\Omega))}\right) + \frac{\alpha}{2}\|z\|^2_{L^2(0,T;L^2(\Omega))}$$

subject to

$$\begin{aligned} \partial_t E - \nabla\times(\mu^{-1}B) + \sigma E &= z_{\rm src} + z \quad \text{in } \Omega\times(0,T) \\ \partial_t B + \nabla\times(\mu^{-1}E) &= 0 \quad \text{in } \Omega\times(0,T) \\ E\times n &= 0. \end{aligned}$$

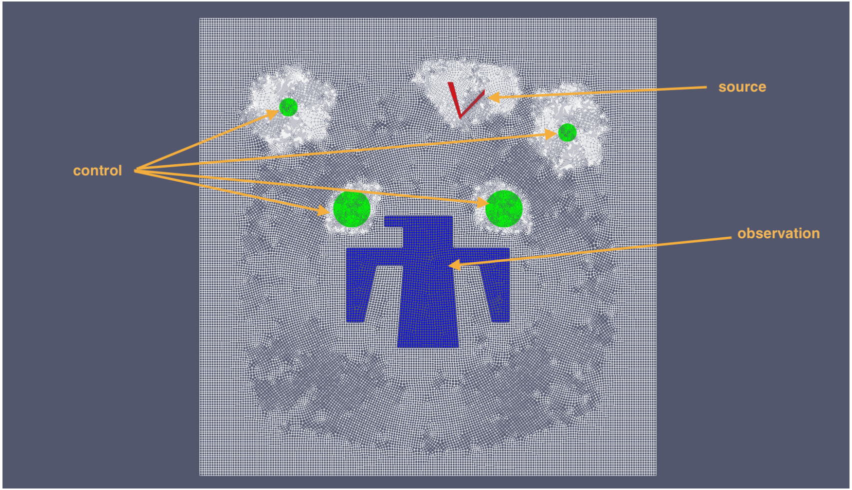
Some new results:

- **Existence of weak solution** for E_0, B_0 in $L^2(\Omega)$ and z, $z_{\rm src}$ in $L^2(0,T;L^2(\Omega))$

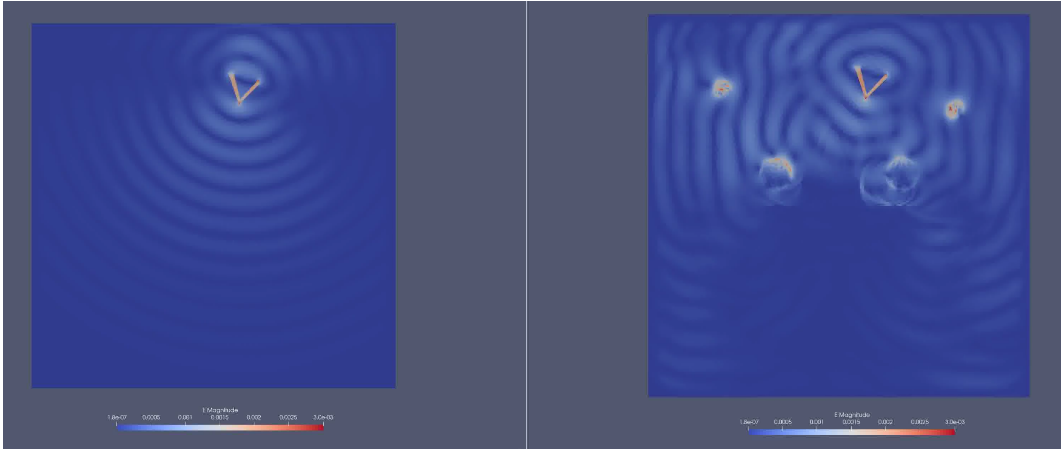
$$\begin{aligned} &E\in H^1(0,T;H_0(\mathsf{curl};\Omega)^*)\cap C([0,T];L^2(\Omega)),\\ &B\in H^1(0,T;H(\mathsf{curl};\Omega)^*)\cap C([0,T];L^2(\Omega))\cap L^\infty(0,T;H^{-1}(\mathsf{div}_0;\Omega)). \end{aligned}$$

- **Convergence of numerical scheme** with (E_h, B_h) in Nedelec and Raviart-Thomas FE spaces, respectively [A., 2025].
- **Optimal control problem:** well-posedness, convergence of discrete scheme, and numerical implementation. [A., Adriazola, Khandelwal, Ridzal, Owusu-Agyemang, 2025]

Example: A New Domain

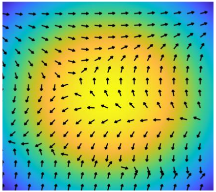


Example: Forward and Optimal Control Problem

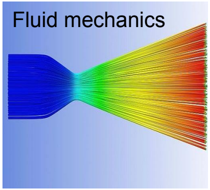


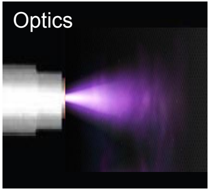
Overview

Objective: Control dynamics of "vector beams" via spatially inhomogeneous polarization

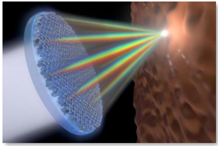


Model light as a fluid:

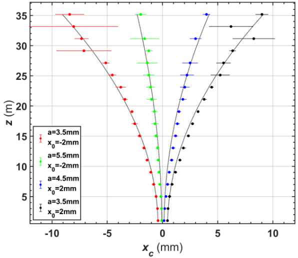




Experimental realization:



Alter beam centroid path by exchange of transverse momentum:

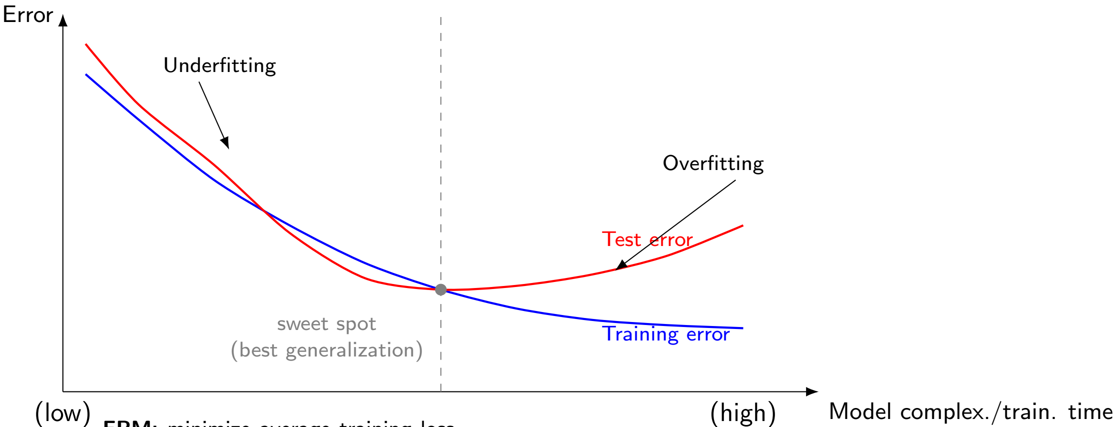


jointly with: Jon Nicols (NRL, DC), Yaw Owusu-Agyemang and Sarswati Shah (GMU)

From True Risk to Empirical Risk Minimization

- **True risk (expected loss):**
$$R(\theta) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\, e(f(x;\theta), y),$$
where $\mathcal{D}$ is the (unknown) data distribution. Here $\mathcal{D}$ is unknown.
[A., Carney, Díaz, Royset (2025)]
- We approximate $R(\theta)$ using the empirical distribution from observed data $\{(x^i, y^i)\}_{i=1}^N$.
- **Empirical risk minimization (ERM):**
$$\min_{\theta=\{W_\ell, b_\ell\}_{\ell=0}^{L-1}} \frac{1}{N}\sum_{i=1}^{N} e(f(x^i;\theta), y^i),$$
subject to:
$$f(x^i;\theta) = (h_{L-1} \circ h_{L-2} \circ \cdots \circ h_0)(x^i), \quad i = 1, \ldots, N.$$
- **Potential issue:** Minimizing empirical risk too aggressively may lead to overfitting— good performance on training data but poor generalization to unseen data.

Empirical Risk Minimization: What Can Go Wrong?



ERM: minimize average training loss.

Caveat: small training error $\not\Rightarrow$ small test error.

Empirical risk minimization (ERM) fits the training set; regularization, validation, and early stopping help avoid the high-complexity overfitting regime.

Supervised Learning: Deep Neural Networks (DNNs)

- Given data $\{(x^i, y^i)\}_{i=1}^N$, solve the learning problem

$$\min_{\theta=\{W_\ell, b_\ell\}_{\ell=0}^{L-1}} \frac{1}{N}\sum_{i=1}^{N} e(f(x^i;\theta), y^i),$$

  subject to: $\quad f(x^i;\theta) = (h_{L-1} \circ h_{L-2} \circ \cdots \circ h_0)(x^i), \quad i = 1, \ldots, N.$

- **Layer definitions:** $\quad h_\ell = \sigma \circ \mathcal{G}_\ell \quad$ (Feedforward), $\qquad h_\ell = I + \tau\,\sigma \circ \mathcal{G}_\ell \quad$ (ResNet), with nonlinear activation σ and affine map $\mathcal{G}_\ell(y) = W_\ell y + b_\ell$.

- **ResNet as ODE:** Each layer update

$$y_\ell = y_{\ell-1} + \tau\,\sigma(W_\ell y_{\ell-1} + b_\ell), \quad \ell = 1, \ldots, L-1,$$

  corresponds to the forward Euler discretization of $\quad d_t y = h(y, \theta), \quad y(0) = x^i.$

- **Continuous learning problem (ODE view):**

$$\min_\theta \frac{1}{N}\sum_{i=1}^{N} e\big(y(T;\theta), y^i\big), \quad \text{subject to } d_t y = h(y,\theta) \quad (\text{or } d_t^\gamma y = h(y,\theta)).$$

[Ruthotto, Haber 2020], [A., Khatri, Löhner, Verma 2020],
[A., Elman, Onwunta, Verma 2023], [A., Díaz, Herberg 2023], [A., Betz, Wachsmuth 2023]