SAND2021-8956PE

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CSRI Summer Proceedings 2021
SAND2021-XXXX

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Verification Testing for Multiphysics Codes

CSRI Summer Proceedings 2021
Presented by: Alexandre Ait Ettajer, RPI
SAND2021-8262 PE

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Verification Testing for Multiphysics Codes

Intern: Alexandre Ait Ettajer, RPI, **Virtual at:** Troy, New York
Mentor: Michael Powell, 1443 (Computational Multiphysics)

Abstract The ALEGRA team is currently updating the code to achieve performance portability on next-generation, heterogeneous HPC architectures. As such, there is a need to measure the resulting changes in accuracy and performance. It is essential to verify that numerical solutions obtained from discretized algorithms converge to correct solutions of the governing equations. This is typically done by computing a sequence of solutions on progressively refined meshes and calculating the rate of convergence of some norm of the solution error. Existing tools to assist developers in verification testing are difficult to use and maintain. The goal of this project is to 1. create an easily useable verification and performance testing toolkit that will compute error norms and convergence rates based on exact or baseline solutions and 2. Perform verification and performance analysis of the next-generation, performance portable code paths in ALEGRA.

Problem Domain	**Technical Approach**	**Mission Application**
Shock Hydrodynamics	Verification Testing	N.D. Components

SAND2021-8262 PE

Preliminary Results & Future Plans

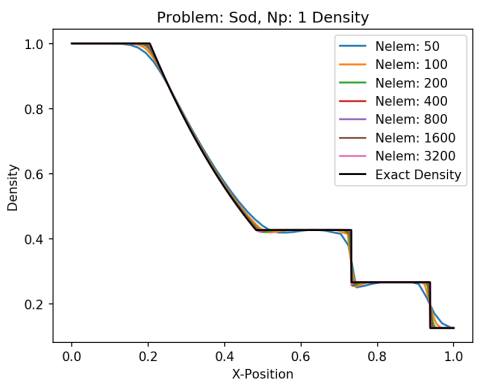
Intern: Alexandre Ait Ettajer, RPI, **Virtual at:** Troy, New York
Mentor: Michael Powell, 1443 (Computational Multiphysics)

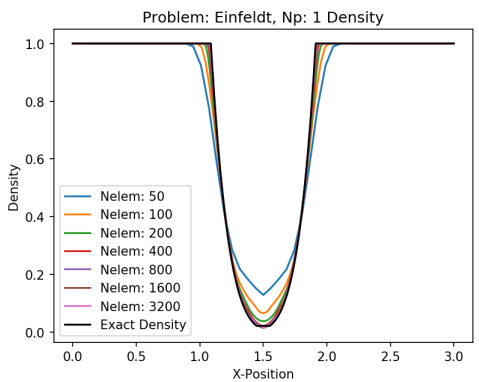
Preliminary Results:

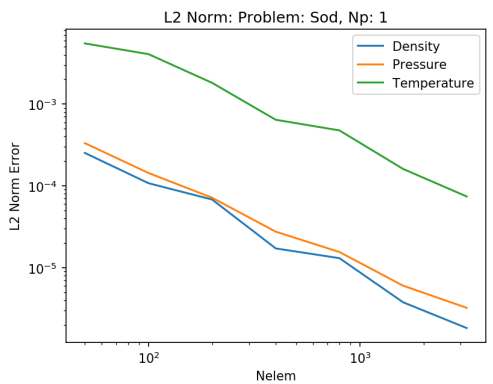
- Convergence Plots for 1D and Quasi-1D Problems, Spatial Plotting for 1D Problems
- Quadrature over field information for Quadrilateral and Hexahedral elements
- Calculation of L_1, L_2, and L_∞ norms on final solutions

Future Plans:

- Perform Comparative analyses between the CPU-only and the performance portable versions of the algorithms
- Add Capability of reading in different file types, ie VTK
- Add Support for Triangular and Tetrahedral elements
- Creation of Convergence Plots for 2D and 3D problems







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Expected information gain estimates and Bayesian optimal experimental design

CSRI Summer Proceedings 2021

Presented by: Terrence Alsup

SAND2021-8679 D

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Expected information gain estimates and Bayesian optimal experimental design

Intern: Terrence Alsup, New York University, **Virtual at:** New York, NY
Mentor: Thomas Catanach, 8579

Abstract Sensor networks are a ubiquitous tool for detecting events in many applications. Here a network of sensors is deployed to gather data for estimating an event's properties. Bayesian optimal experimental design (OED) provides a framework for optimizing the configuration of the network of sensors. In particular, the sensors are configured to maximize the expected information gain (EIG). For a given sensor configuration, the EIG takes the form of a nested expectation and therefore is computationally intensive to accurately estimate by sampling. For the Bayesian optimization of the network we use a resampling method to estimate the uncertainty in the EIG estimate. We find that, in practice, this resampling method provides an upper bound on the true error of the EIG estimate.

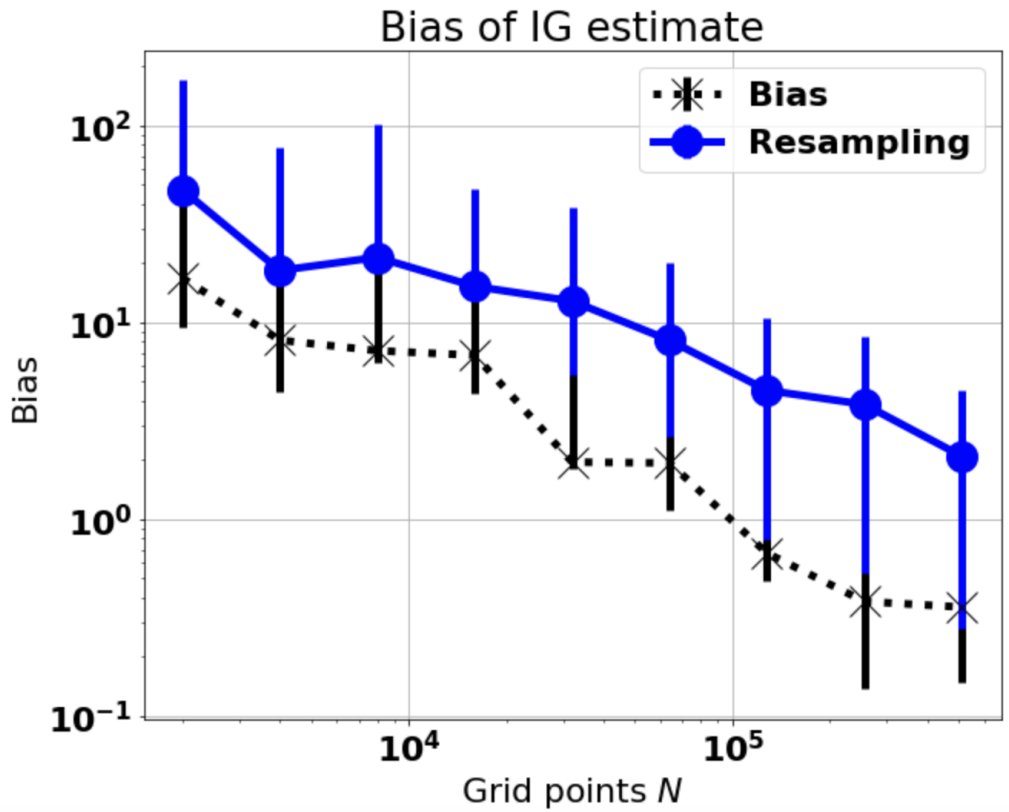
Problem Domain	**Technical Approach**	**Mission Application**
Network optimization	Bayesian optimal experimental design	Seismic monitoring

SAND2021-8679 D

Preliminary results

Intern: Terrence Alsup, New York University, **Virtual at:** New York, NY
Mentor: Thomas Catanach, 8759

Our preliminary experiments have shown that our resampling method provides an upper bound for the error when estimating information gain (IG) on a 4D toy problem.



Future work...

- Extend this to the seismic OED problem
- Obtain a tighter bound if possible (more efficient)
- Derive a trade-off between accuracy of estimate and cost

Importance Sampling in Bayesian OED for Sensor Placement

CSRI Summer Proceedings 2021

Presented by: Jake Callahan

SAND2021-8767 D

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Importance Sampling in Bayesian OED for Sensor Placement

Intern: Jake Callahan, Brigham Young University, **Virtual at:** Provo, Utah
Mentor: Thomas Catanach, 8759 (Extreme-scale DS & Analytics)

Abstract The goal of Bayesian optimal experimental design (OED) is to find experiments that reduce uncertainty in an optimal way. We use Bayesian OED to find optimal sensor configurations for detecting events of interest. It is useful to be able to easily sample from different priors that represent different situations in which these events are manifest. Some such priors are irregular and difficult to sample from. Importance sampling can be used to sample those distributions from which sampling is easier while still obtaining good approximations of the parameter of interest. In this work we implement an importance sampling method to approximate expected information gain (EIG) and examine the effects of importance distribution choice on the quality of EIG approximation.

Problem Domain

Bayesian OED

Technical Approach

Importance Sampling

Mission Application

Seismic Monitoring

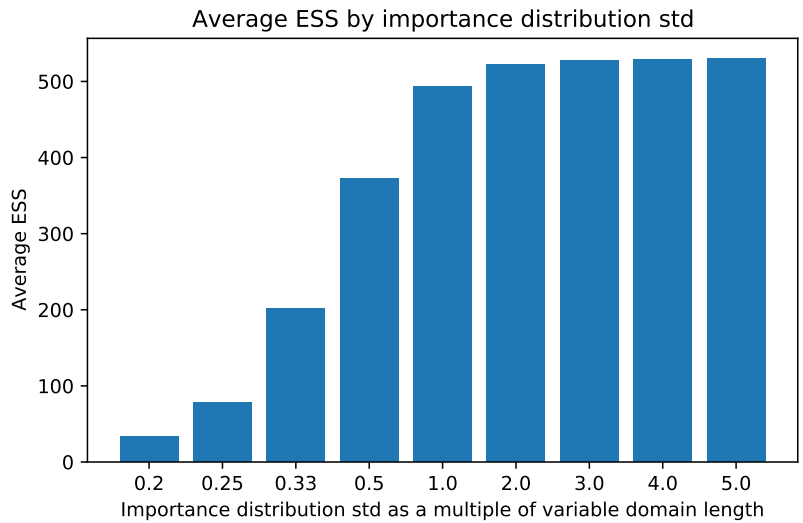
SAND2021-8767 D

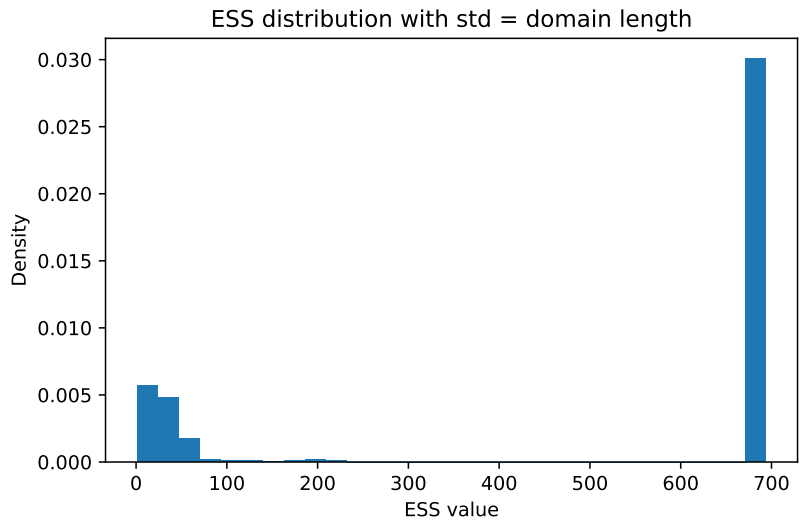
Importance Sampling in Bayesian OED for Sensor Placement preliminary results

Intern: Jake Callahan, Brigham Young University, **Virtual at:** Provo, Utah
Mentor: Thomas Catanach, 8759 (Extreme-scale DS & Analytics)

Our preliminary experiments have shown that with a sufficiently wide importance distribution we can achieve reasonable results on relatively small sample size (8192 samples), as measured by Effective Sample Size (ESS).

Next, we will investigate the effects of fault line-shaped priors on sensor placement.





SAND2021-8767 D

Moment Propagation in Discrete -Time Systems

CSRI Summer Proceedings 2021

Presented by: Thomas Dean

SAND2021-8749 PE

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Moment Propagation in Discrete -Time Systems

Intern: Thomas Dean, University of Wyoming, **Virtual at:** Laramie, Wyoming
Mentor: Edgar Galvan, 8754 Department of Quant Modeling & Analysis

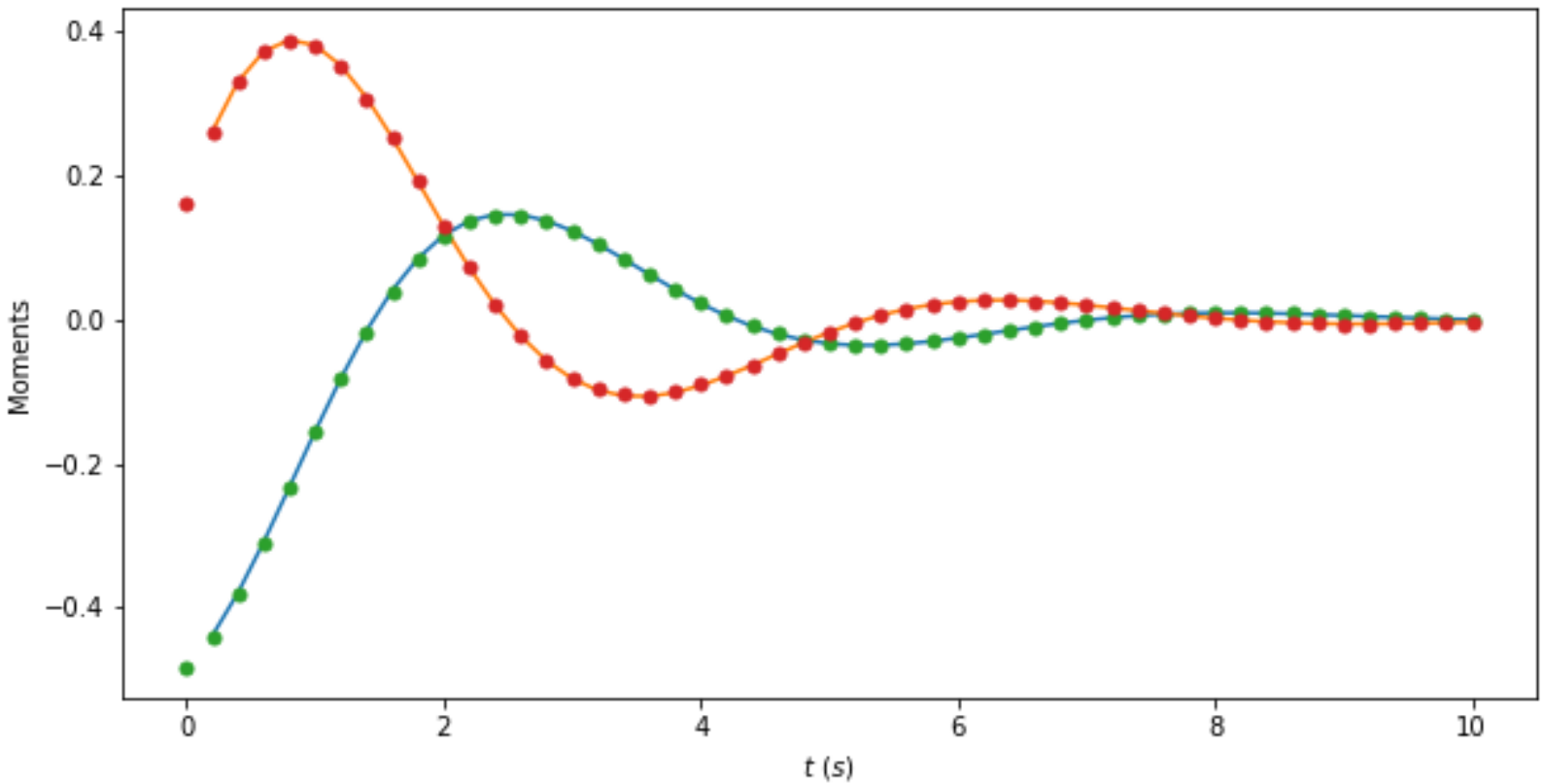
Abstract We discuss the study of uncertainty quantification in nonlinear dynamical systems where we use the Koopman Operator and DMD to transform the system into an infinite dimensional linear system. It has been shown that the first moment, which is the expected value, of a dynamical system can be propagated forward in time so that we can understand the expected value of the system at any future time. We propose a method for propagating the second moment, also known as the variance, with the hope that this approach extends to higher order moments. To verify that our approach works, we compare our results with the Monte-Carlo method. The proposed Koopman method is much faster compared to Monte-Carlo because the main computation required is matrix multiplication.

Problem Domain	**Technical Approach**	**Mission Application**
Uncertainty Quantification	Moment propagation	Electrical Simulation

SAND2021-8749 PE

Moment propagatin in Discrete -Time Systems: preliminary results

Intern: Thomas Dean, University of Wyoming, **Virtual at:** Laramie, Wyoming
Mentor: Edgar Galvan, 8754 Department of Quant Modeling & Analysis



SAND2021-8749 PE

Partitioned ROM-FEM model coupling for transmission problems

CSRI Summer Proceedings 2021

Presented by: Amy de Castro

SAND2021-8372 A

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Partitioned ROM-FEM model coupling for transmission problems

Intern: Amy de Castro, Clemson University, **Virtual at:** Clemson, SC
Mentors: Paul Kuberry, 1442 Comp. Math | Pavel Bochev, 1400 Computing Research

Abstract Application of reduced order modeling (ROM) on select subdomains can help to increase the computational efficiency of Multiphysics simulations. We develop a partitioned scheme for a model interface problem which couples a ROM with a conventional finite element method. The proper orthogonal decomposition (POD) approach is implemented to construct a low-dimensional reduced basis on half the domain and solve the subdomain problem in terms of this basis. The ROM solution is then coupled to the FEM solution using a Lagrange multiplier representing the interface flux. The multiplier at the current time step can be expressed as an implicit function of the state solutions through a Schur complement. As a result, application of an explicit time integration scheme decouples the subdomain problems, allowing their independent solution for the next time step.

Problem Domain	**Technical Approach**	**Mission Application**
Coupled multiphysics	Reduced order modeling	Climate; multimaterial simulations

SAND2021-8372 A

Partitioned ROM-FEM model coupling for transmission problems

Intern: Amy de Castro, Clemson University **Virtual at:** Clemson, SC
Mentors: Paul Kuberry, 1442 Comp. Math | Pavel Bochev, 1400 Computing Research

Step 1: Use a Lagrange multiplier to couple the ROM & FEM representations on the subdomains. Enforcing continuity of time derivatives yields an Index-1 DAE:

$$\begin{bmatrix} \tilde{U}^T M_1 \tilde{U} & 0 & \tilde{U}^T G_1^T \\ 0 & M_2 & -G_2^T \\ G_1 \tilde{U} & -G_2 & 0 \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{\varphi}}_{\boldsymbol{R}} \\ \dot{\Phi}_2 \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \tilde{U}^T \mathrm{f}_1(\tilde{U}\boldsymbol{\varphi}_{\boldsymbol{R}} + \Phi_{10}) \\ \mathrm{f}_2(\Phi_2) \\ 0 \end{bmatrix}$$

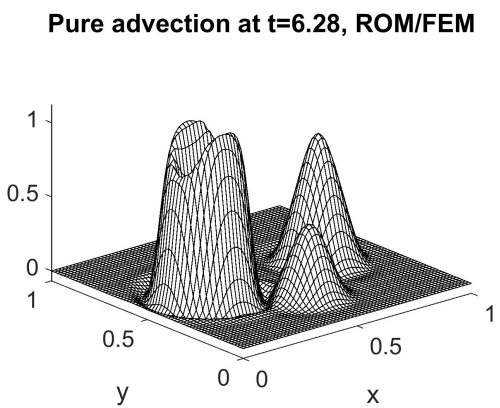
Step 2: Explicit time integration decouples the Index-1 DAE into 2 independent ODEs:

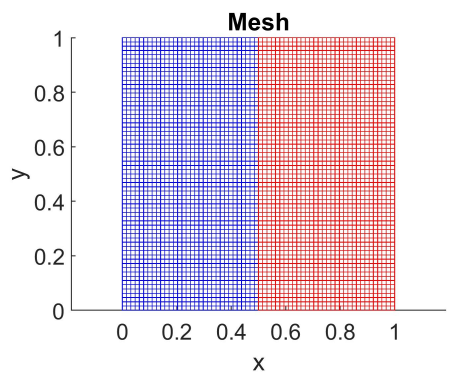
$$(\tilde{U}^T M_1 \tilde{U}) D_t^n(\boldsymbol{\varphi}_{\boldsymbol{R}}) = \tilde{U}^T \boldsymbol{f}_1^{\boldsymbol{n}} - \tilde{U}^T G_1^T \boldsymbol{\lambda}^{\boldsymbol{n}}$$

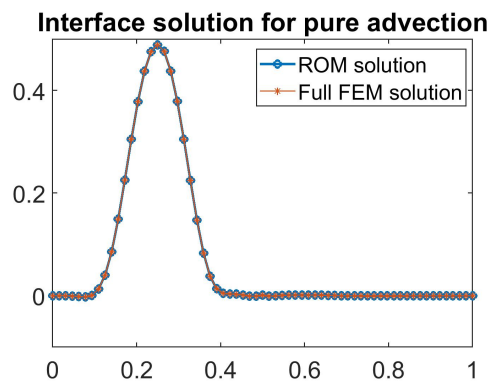
$$M_2 D_t^n(\Phi_2) = \boldsymbol{f}_2^{\boldsymbol{n}} + G_2^T \boldsymbol{\lambda}^{\boldsymbol{n}}$$

Step 3: Use a Schur complement to solve for $\boldsymbol{\lambda}^{\boldsymbol{n}}$:

$$\left(G_1 \tilde{U} (\tilde{U}^T M_1 \tilde{U})^{-1} \tilde{U}^T G_1^T + G_2 M_2^{-1} G_2^T \right) \boldsymbol{\lambda}^{\boldsymbol{n}} = G_1 \tilde{U} (\tilde{U}^T M_1 \tilde{U})^{-1} \tilde{\boldsymbol{f}}_1^{\boldsymbol{n}} - G_2 M_2^{-1} \tilde{\boldsymbol{f}}_2^{\boldsymbol{n}}$$







21-8372 A

Nonlocal operator learning with Uncertainty Quantification

CSRI Summer Proceedings 2021

Presented by: Yiming Fan

SAND2021-8757 D

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Nonlocal operator learning with Uncertainty Quantification

Intern: Yiming Fan, Lehigh Univeristy, **Virtual at:** Bethlehem, PA
Mentor: Marta D'Elia, 8754 Department of Quantitative Modeling and Analysis

Abstract The goal of this work is to develop a Bayesian framework to characterize the uncertainty of material response when using a nonlocal, homogenized model to describe wave propagation through heterogeneous, disordered materials. Our approach is based on an operator regression technique combined with Bayesian optimization. Specifically, we use a MCMC method to identify the probability distribution of the nonlocal constitutive law that embeds the material's properties.

Problem Domain	**Technical Approach**	**Mission Application**
Nonlocal models,	Bayesian inference,	Wave propagation
Data-driven learning	MCMC	

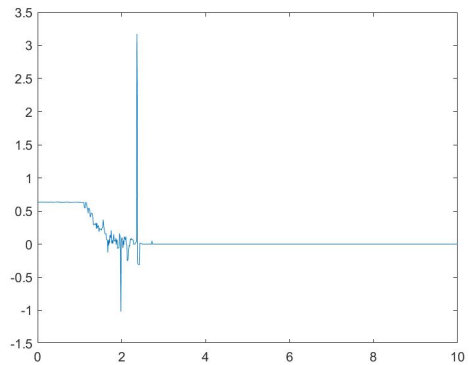
SAND2021-8757 D

Preliminary results

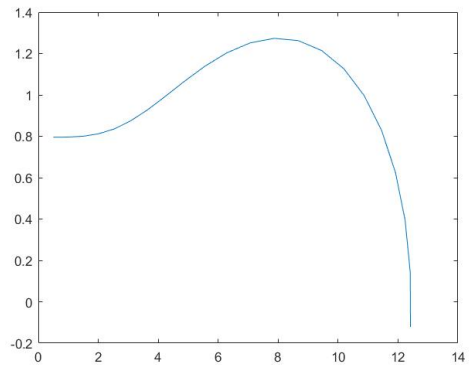
Intern: Yiming Fan, Lehigh Univeristy, **Virtual at:** Bethlehem, PA
Mentor: Marta D'Elia, 8754 Department of Quantitative Modeling and Analysis

When learning material properties in the context of wave propagation, it is fundamental to recover the group wave velocity (GWV) accurately. The GWV for a disordered microsturcture could be very oscillatory, see Figure (a) where the average GWV over XX samples is reported. This curve is used in our first deterministic step to estimate the best nonlocal kernel that matches such GWV.

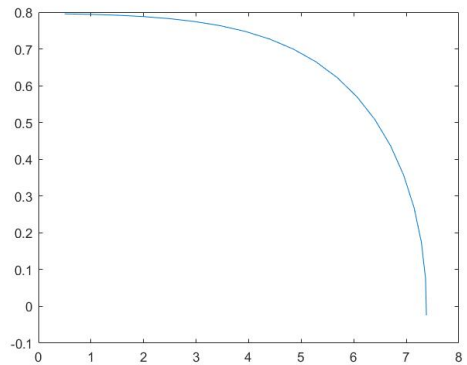
In our first experiment with fix all parameters the (boundary conditions and loadings) and only change microstructure from sample to sample in the training data set. The learnt parameters, and hence the learnt GWV, are very sensitive to the Tikhonov regularization parameter used in the optimization. This is likely due to the lack of variability in the training set. Thus, we will next consider a wider and more diverse data set that includes loadings of varying frequencies.



(a) Average group velocity for disordered material



(b) Learning result using regularization parameter 0.01



(c) Learning result using regularization parameter 0.1

SAND2021-8757 D

Benchmarking Quantum Algorithms with Neural Networks

CSRI Summer Proceedings 2021

Presented by: Collin Frink

SAND2021-8758 D

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Benchmarking Quantum Algorithms with Neural Networks

Intern: Collin Frink, University of Wisconsin, Madison, **Virtual at:** Shoreview, MN
Mentor: Andrew Baczewski, 1425 Department of Quantum Computing

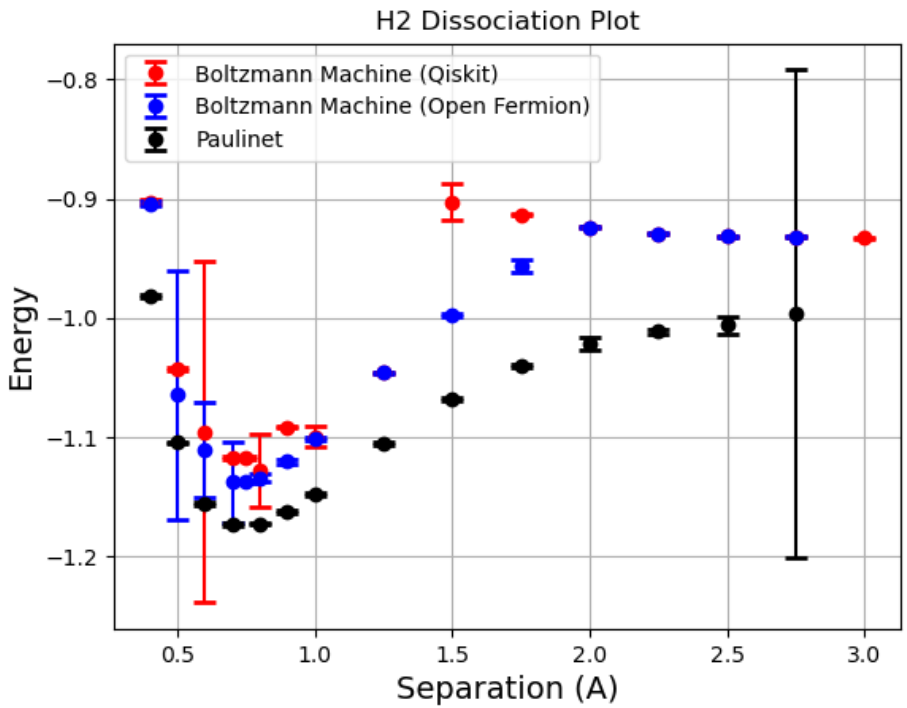
Abstract Quantum computers are an exciting technology that promises to revolutionize fields in physics, computer science, biology, etc. Thus there is motivation to develop and benchmark algorithms for quantum computers as the physical technology develops. In order to do so, it is useful to understand the capabilities of classical computers to perform similar tasks in which quantum algorithms are theorized to be effective. Recently, some of these classical methods have adopted neural networks to increase computational efficiency. The goal of this project, then, is to determine the effectiveness and efficiency of a variety of neural networks. More specifically, the performance of simpler network structures (Restricted Boltzmann machines) is compared to that of more complex network structures (such as Paulinet and Ferminet) in solving classical physics problems such as dissociation energies.

Problem Domain	**Technical Approach**	**Mission Application**
Quantum Chemistry	Neural Networks	Quantum Technology

SAND2021-8758 D

H2 Dissociation Energy

Intern: Collin Frink, University of Wisconsin, Madison, **Virtual at:** Shoreview, MN
Mentor: Andrew Baczewski, 1425 Department of Quantum Computing



Above: solutions to the H2 dissociation energy found by two Restricted Boltzmann machines (5 mins) and a CNN based network; Paulinet (3 hrs).

Next, we will further our investigations into the efficiency and effectiveness of all of the previously listed neural networks through hyper-parameter tuning, and deeper examinations of computational efficiency. Computationally harder problems, such as dissociation energies of larger molecules, can also be used to benchmark each network. Other network structures (including deeper artificial neural networks with more layers than a Boltzmann machine) are another point of interest.

SAND2021-8758 D

Split Bregman optimizer for online generalized CP tensor decomposition

CSRI Summer Proceedings 2021

Presented by: Kyle Gilman

SAND2021-8805 D

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Split Bregman optimizer for online generalized CP tensor decomposition

Intern: Kyle Gilman, University of Michigan, **Virtual at:** Ann Arbor, MI
Mentor: Eric Phipps, Hemanth Kolla, 1465 Department of Scalable Algorithms

Abstract Rank-R online CP tensor decomposition for general losses requires solving the following problem each time new multiway data arrives:

$$\min_{c_t} \sum_{i \in \Omega} f\left(x_{it}, (\mathbf{\Pi} c_t)_i\right) + \frac{\mu}{2}\|c_t\|_2^2, \quad \mu > 0, \tag{1}$$

where x_{it} is the i^{th} entry of the d-way data (hyper)slice $\mathcal{X}_t$ at time t, $\mathbf{\Pi} = A^{(1)} \odot \cdots \odot A^{(d)}$ is the Khatri-Rao product of the non-time-dependent tensor modes, $c_t \in \mathbb{R}^R$ are the weights, and $f(\cdot,\cdot) : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is the negative log-likelihood of a chosen statistical distribution.

Optimizing (1) can be fairly challenging, and gradient descent may be slow to converge and challenging to tune. We present a split Bregman approach using fast majorization-minimization techniques for difference of convex statistical losses.

Problem Domain

Tensor Decompositions

Technical Approach

Generalized CPD

optimization

Mission Application

Computer network

anomaly detection

SAND2021-8805 D

Preliminary results

Intern: Kyle Gilman, University of Michigan, **Virtual at:** Ann Arbor, MI

Mentor: Eric Phipps, Hemanth Kolla, 1465 Department of Scalable Algorithms

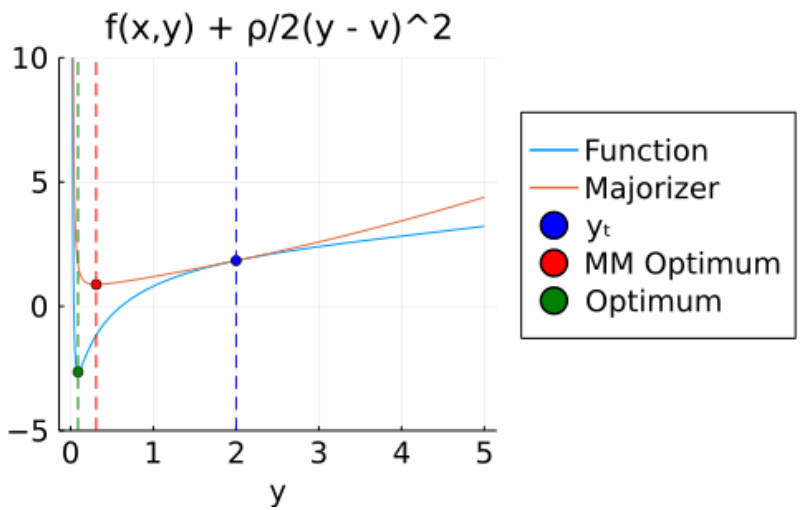
Split Bregman of (1): the most challenging step in the optimization involves solving separable, elementwise problems of the following form for each ADMM iteration:

$$\text{prox}_{\frac{1}{\rho}f}(v) = \underset{y}{\text{argmin}}\, f(x,y) + \frac{\rho}{2}(y-v)^2, \quad \rho > 0. \tag{2}$$

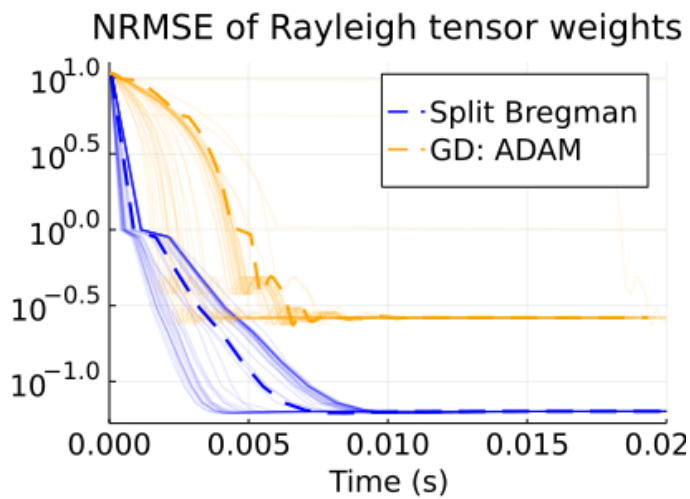
Observation: $f(x,y) = \breve{l}(x,y) + \hat{l}(x,y) := \text{convex}(x,y) + \text{concave}(x,y)$ for most loss functions of interest.

Minimize a Difference of Convex (DoC) majorizer:

$y_{t+1} = \text{argmin}_y\, \breve{l}(x,y) + \hat{l}(x,y_t) + \nabla\hat{l}(x,y_t)(y-y_t) \Rightarrow$ fast and simple updates!



(a) DoC majorizer for proximal operator with Rayleigh $f(\cdot,\cdot)$.



(b) Experiments over 50 random initializations to solve (1).

SAND2021-8805 D

The Impact of Continental Scale Ice-Sheet Model Error on Inferred Parameter Uncertainties

CSRI Summer Proceedings 2021

Presented by: Tucker Hartland

SAND2021-8272 A

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The Impact of Continental Scale Ice-Sheet Model Error on Inferred Parameter Uncertainties

Intern: Tucker Hartland, University of California, Merced, **Virtual at:** Merced, CA
Mentor: Mauro Perego, 1442 Department of Computational Mathematics

Abstract Various spatially distributed ice-sheet model parameters are practically inaccessible to measurement, such as the basal friction parameter field. The basal friction field determines how free the ice-sheet is to slide over the underlying bedrock that supports it, the rate at which the ice-sheet flows out to the ocean and ultimately the contribution of the ice-sheet to sea-level rise. Given how the basal friction field impacts model predictions of future sea-level rise it is critical that we can efficiently infer it from surface velocity measurement data as well as obtain accurate uncertainty estimates of the inference. No model is perfect and so in this work, model errors are estimated to improve the accuracy of quantified inferred parameter uncertainties.

Problem Domain	**Technical Approach**	**Mission Application**
Bayesian inverse problems	Bayesian approx. error	Geosciences

SAND2021-8272 A

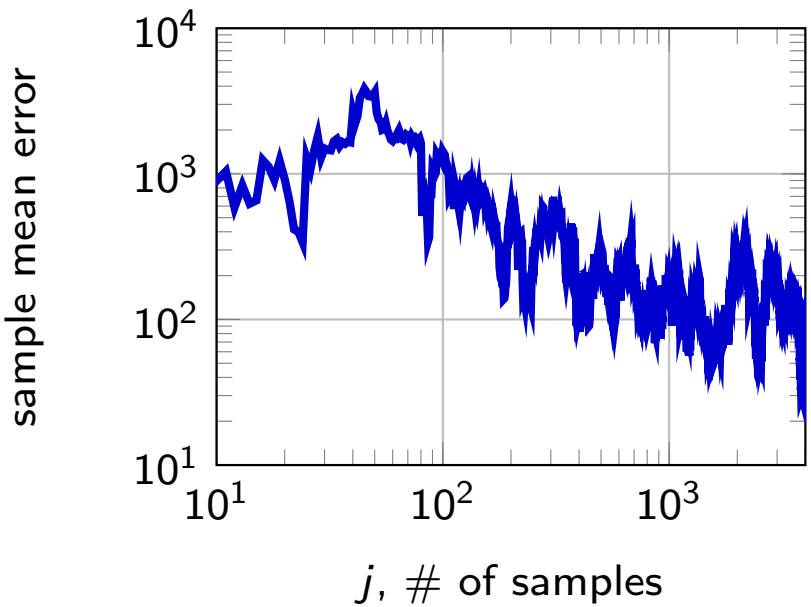
Preliminary Results

Intern: Tucker Hartland, University of California, Merced, **Virtual at:** Merced, CA
Mentor: Mauro Perego, 1442 Department of Computational Mathematics

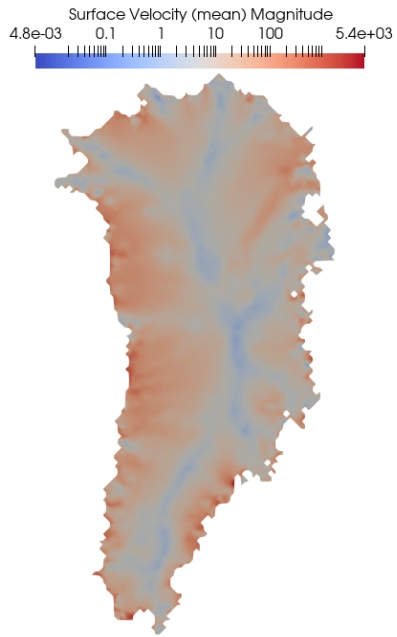
To improve the inference of the parameter $\boldsymbol{\beta}$, by accounting for model error due to an uncertain secondary parameter $\boldsymbol{\phi}$, we sample the model discrepancy

$$\boldsymbol{\varepsilon} = \boldsymbol{\mathcal{F}}(\boldsymbol{\beta}, \boldsymbol{\phi}) - \boldsymbol{\mathcal{F}}(\boldsymbol{\beta}, \boldsymbol{\phi}_*),$$

and build a Gaussian approximation of the prior model discrepancy.



- $\boldsymbol{\mathcal{F}}$ – parameter to model prediction map,
- $\boldsymbol{\beta}, \boldsymbol{\phi}$ – discretized primary and secondary Gaussian parameter fields with means $\boldsymbol{\beta}_*, \boldsymbol{\phi}_*$



Greenland ice-sheet model flow prediction, $\boldsymbol{\mathcal{F}}(\boldsymbol{\beta}_*, \boldsymbol{\phi}_*)$

SAND2021-8272 A

Survey of dynamic contact algorithms

CSRI Summer Proceedings 2021

Presented by: Jonathan Hoy

SAND2021-8753 PE

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Survey of dynamic contact algorithms

Intern: Jonathan Hoy, University of Southern California, **Virtual at:** Los Angeles, CA
Mentor: Irina Tezaur, 08754 Department of Quantitative Modeling and Analysis

Abstract Contact problems have a wide range of application in engineering sciences. Such problems are inherently non-linear due to the presence kinematic constraints that prevent interpenetration of the bodies in contact. As such, they can be particularly difficult to solve and careful consideration must be given in the formulation of solution algorithms. A novel method based on the Schwarz alternating method is compared to established approaches such as the penalty, lagrange multiplier, and augmented lagrangian method. The canonical problem used for comparison is the impact of two rods with identical properties traveling at equal velocities towards each other. The numerical results from each algorithm are compared to the analytical solution to assess performance.

Problem Domain	**Technical Approach**	**Mission Application**
Finite Element Analysis	Dynamic Contact	Solid Mechanics

SAND2021-8753 PE

Survey of dynamic contact algorithms: preliminary results

Intern: Jonathan Hoy, University of Southern California, **Virtual at:** Los Angeles, CA
Mentor: Irina Tezaur, 08754 Department of Quantitative Modeling and Analysis

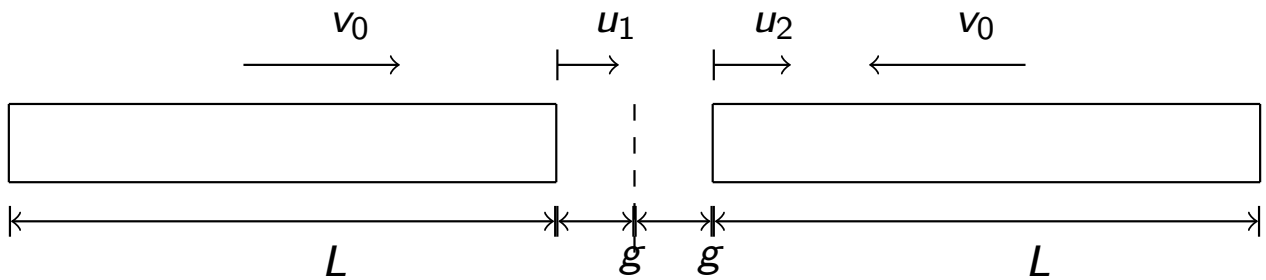
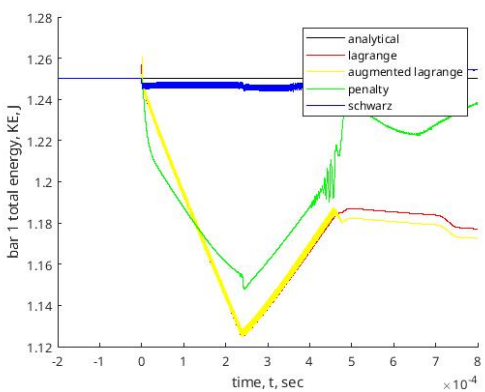
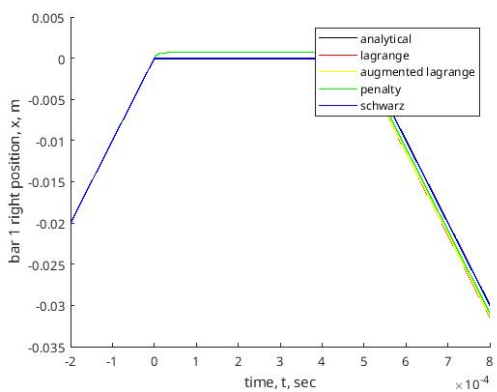


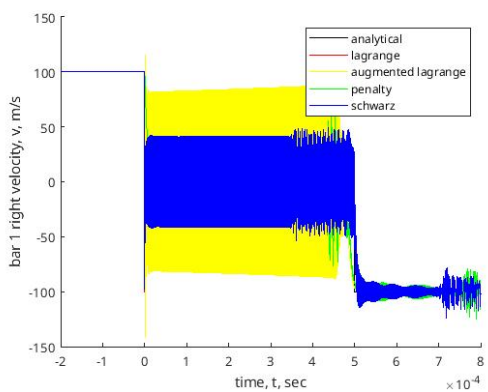
Illustration of problem setup for 1-D impact

The parameters used by each method are shown in the table below

N_x	Δt	ρ	E	v_0	L	g	A
200	1.0e-7	1.0e3	1.0e9	1.0e2	0.25	0.02	1.0e-6







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Reduced-order modeling for uncertainty quantification

CSRI Summer Proceedings 2021

Presented by: Ruhui Jin

SAND2021-8568 P

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[Reduced-order modeling for uncertainty quantification]

Intern: Ruhui Jin, University of Texas at Austin, **Virtual at:** Austin, Texas.
Mentor: Eric Parish, 8759, Extreme Scale Data Science & Analytics.
Francesco Rizzi, NexGen Analytics.

Abstract Uncertainty quantification (UQ) for parametrized systems is crucial in a wide range of computational science and engineering applications. Performing computations on full-order models becomes infeasible in large-scale systems with high-dimensional uncertainties. Reduced-order modeling (ROM) is a promising technique to tackle this computational bottlebeck. However, existing ROM techniques often achieve dimension reduction only on the spatial domain. In this work, we study novel space-time model reduction methods combined with classical UQ propagation approaches such as stochastic Galerkin and Monte-Carlo. We utilize the proposed method to solve advection-diffusion PDEs with random parameters. Our result shows that the methodology can boost significant speed-up in practice.

Problem Domain

UQ, predictive simulations.

Technical Approach

Reduced-order modeling, stochastic UQ propagation methods.

Mission Application

Climate modeling, hypersonic aerodynamics.

SAND2021-8568 P

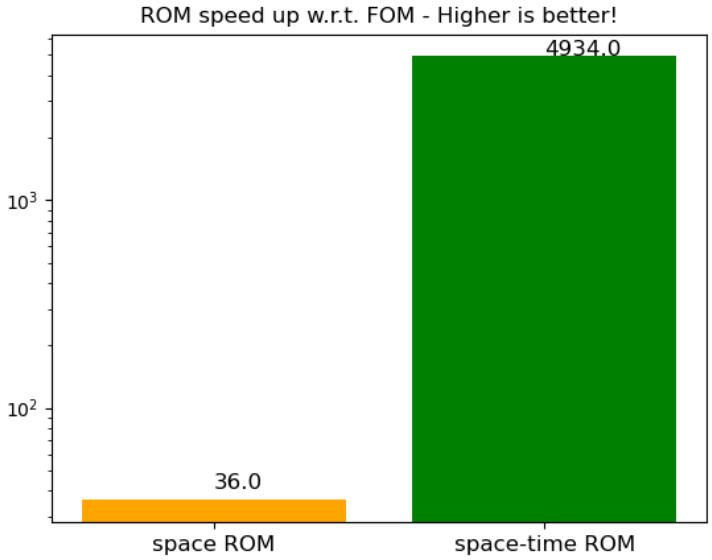
Preliminary results

Preliminary experiments have shown that space-time ROM has high **computation efficiency**, without the loss of accuracy and convergence property.
Given a 1D advection-diffusion problem,

$$\frac{\partial u}{\partial t} + c\,\frac{\partial u}{\partial x} = \nu\,\frac{\partial u^2}{\partial x^2} + g, \tag{1}$$

where random coefficients: $c \sim \mathcal{N}(1, 0.15)$ and $\nu \sim U[0.01, 0.02]$.

Next, we will investigate space-time ROM approach on higher dimensional parametrized systems.



Learning Transferable DFT Neural Network Surrogates

CSRI Summer Proceedings 2021

Presented by: Kyle Lennon

SANDSAND2021-8771 D

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[Learning Transferable DFT Neural Network Surrogates]

Intern: Kyle Lennon, MIT, **Virtual at:** Cambridge, MA
Mentor: Sivasankaran Rajamanickam, 1465 Department of Scalable Algorithms

Abstract Density functional theory (DFT) is widely used to compute properties of many-body systems from first principles, and often serves as an intermediate step to computing forces on atomic nuclei in molecular dynamics (MD) simualtions. However, DFT calculations are computationally intensive, and their cost becomes prohibitive for large systems or long MD simulations. Recently, efforts to circumvent expensive DFT calculations by learning system-specific neural network surrogates have been met with some success. Still, these surrogates require the generation of *ab initio* training data and long training times for every individual system and thermodynamic state. Here, we investigate whether this approach can be made more widely applicable by leveraging modern machine learning techniques, such as meta-learning or Bayesian approaches, to produce surrogate models that transfer between systems and states, or adapt quickly without the need for extensive training.

Problem Domain	**Technical Approach**	**Mission Application**
Meta/Transfer Learning	Information Bottlenecking	Molecular Simulations

SANDSAND2021-8771 D

Efficient Computation of Higher Order Moment Tensor

CSRI Summer Proceedings 2021

Presented by: Zitong Li

SANDSAND2021-8822 D

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Efficient Computation of Higher Order Moment Tensor

Intern: Zitong Li, Wake Forest University, **Virtual at:** Winston Salem, NC
Mentor: Hemanth Kolla, 8753 Department of Scalable Modeling & Analysis

Abstract The tensor decomposition of the cumulant tensor of time series data can be used to effectively detect and analyze anomalies. However, computing the cumulant tensor can be very expensive. One of the most expensive steps is to compute the moment Tensor. The current state-of-art algorithm takes advantage of the symmetric nature of the moment tensor by dividing it into smaller cubic tensor blocks and only compute the blocks with unique values and thus reducing computation. We designed a new algorithm that poses the computation of the moment tensor in terms of matrix operations (Khatri-Rao product and matrix multiplication). Because this approach is much more cache efficient, we were able to achieve a 5x speedup over the state-of-art with typical input data dimensions on a single processor. Ongoing efforts include implementing this algorithm with Kokkos to make it scalable.

Problem Domain	**Technical Approach**	**Mission Application**
Moment Tensor Computation	Khatri-Rao product	Combustion

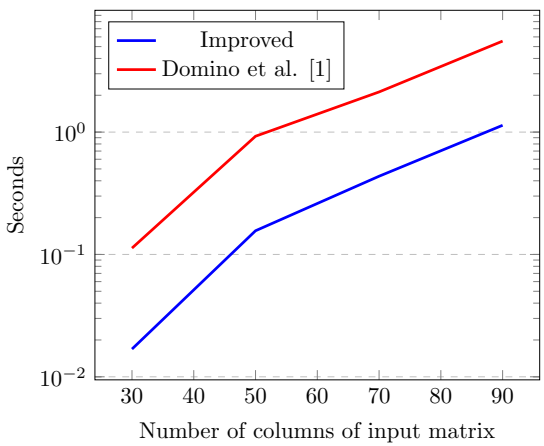
SANDSAND2021-8822 D

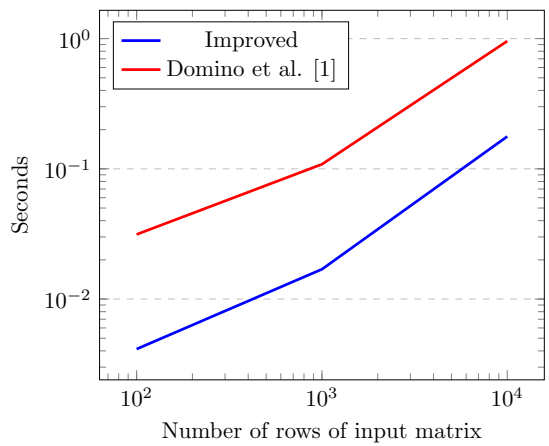
Efficient Computation of Higher Order Moment Tensor

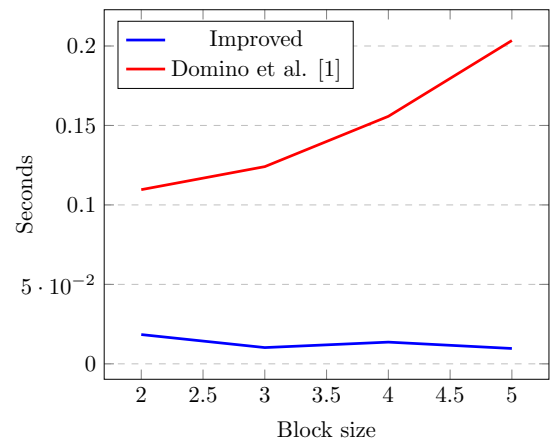
Intern: Zitong Li, Wake Forest University, **Virtual at:** Winston Salem, NC
Mentor: Hemanth Kolla, 8753 Department of Scalable Modeling & Analysis

The following experiment is ran with synthetic random matrices (1000x30 with a block size of 2). Controlling other parameters, we varied the number of columns and rows of the input matrix and the block size. Our performance is in blue while the red lines represent that of the existing approach by Domino et al.[1].

As we can see, the speedup is consistent around 5x across the different number of columns and rows. The block size also has an impact on the performance. Our approach prefers a larger block size, which results in less saving in terms of memory. However, we are outperforming the existing approach even with smaller block sizes.







[1] K. Domino, P. Gawron, and Ł. Pawela, "Efficient Computation of Higher-Order Cumulant Tensors," SIAM J. Sci. Comput., vol. 40, no. 3, pp. A1590–A1610, Jan. 2018, doi: 10.1137/17M1149365.

SANDSAND2021-8822 D

pMEMCPY: an efficient I/O library for PMEM

CSRI Summer Proceedings 2021

Presented by: Luke Logan

SAND2021-8666 C

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[pMEMCPY: an efficient I/O library for PMEM]

Intern: Luke Logan, Illinois Institute of Technology, **Virtual at:** Chicago, IL
Mentor: Jay Lofstead, 1423 Department of Scalable Systems Software

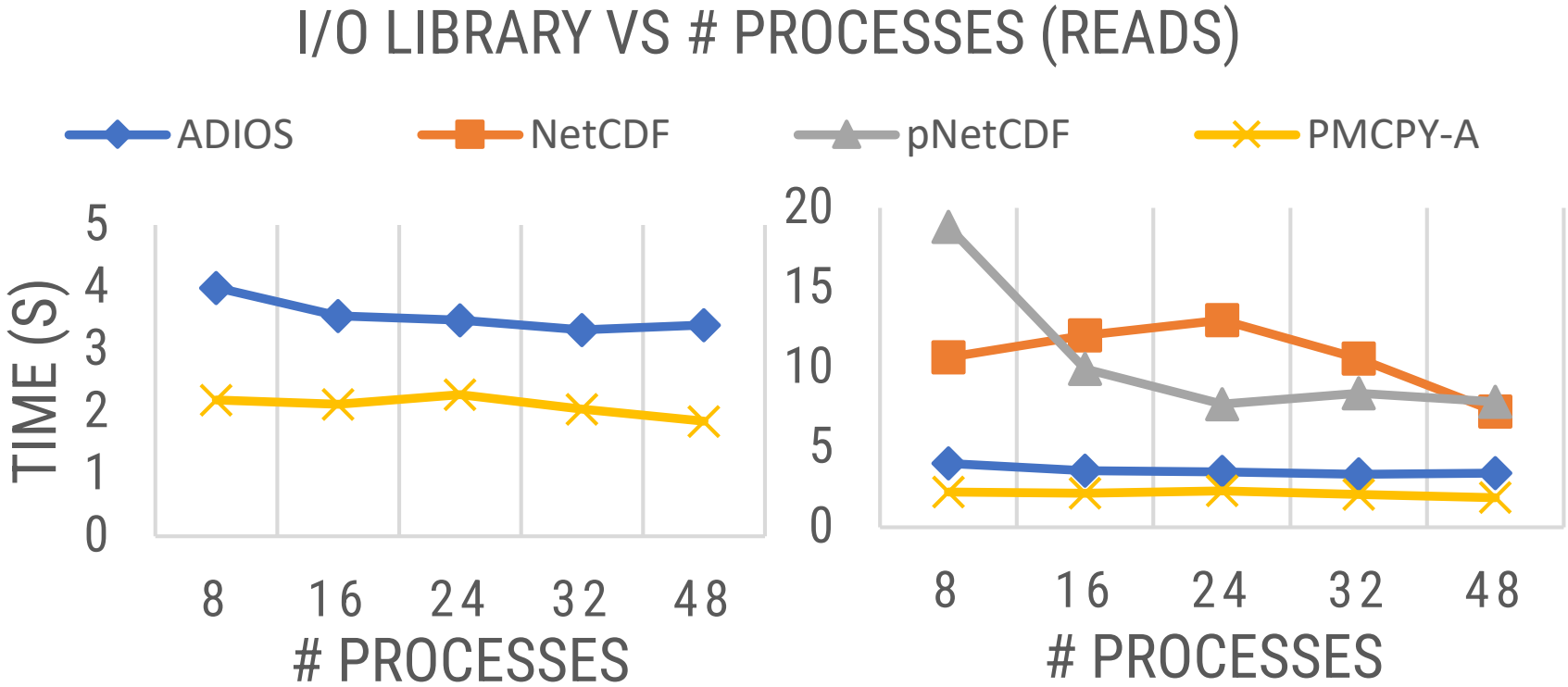
Abstract Persistent memory (PMEM) can achieve comparable performance to DRAM while providing significantly more capacity. This has made the technology compelling as an expansion to main memory. Rethinking PMEM as storage devices can offer a high performance buffering layer for HPC applications to temporarily, but safely, store data. However, modern parallel I/O libraries, such as HDF5 and pNetCDF, are complicated and introduce significant software and metadata overheads when persisting data to these storage devices, wasting much of their potential. In this work, we explore the potential of PMEM as storage through pMEMCPY: a simple, lightweight, and portable I/O library for storing data in persistent memory. We demonstrate that our approach is up to 2x faster than other popular parallel I/O libraries under real workloads.

Problem Domain	**Technical Approach**	**Mission Application**
Resource Utilization	Memory Mapping	Supercomputing

SAND2021-8666 C

[Experimental Results]

Intern: Luke Logan, Illinois Institute of Technology, **Virtual at:** Chicago, IL
Mentor: Jay Lofstead, 1423 Department of Scalable Systems Software



pMEMCPY is 5x faster than pNetCDF and NetCDF by avoiding network communications and data copying costs. pMEMCPY is 2x faster than ADIOS since it avoids data copying costs required by POSIX.

SAND2021-8666 C

Trajectory Anomaly Detection

CSRI Summer Proceedings 2021

Presented by: Maxwell Low

SAND2021-8778 PE

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Trajectory Anomaly Detection

Intern: Maxwell Low, Purdue University, **Virtual at:** Albuquerque, New Mexico
Mentor: Andrew Wilson , 1461 Department of Scalable Analysis and Visualization

Abstract A trajectory is a time ordered collection of positional markers: sets of latitude, and longitude with adjoining time stamps. Nearly every moving object traces a path that could be studied as a trajectory. The following examples are derived from aircraft and maritime trajectories.

Problem Domain
Outlier Detection

Technical Approach
Density based clustering

Mission Application
Geo-spatial analysis

To detect anomalys we use is a density based spatial clustering algorithm, which assigns trajectories to groups based on their characteristics. These characteristics are identifying aggregates from each trajectory, called features. Some features are: a flights average altitude or velocity, its total amount of turning, or a quantification of how curved/straight a flight is. Analyzing the groups created by clustering, based on features, allow for the determination of patterns and commonalities among trajectories. Any trajectories which do not have a group are anomalies and warrant further study.

SAND2021-8778 PE

Preliminary Results

Intern: Maxwell Low, Purdue University, **Virtual at:** Albuquerque, New Mexico
Mentor: Andrew Wilson, 1461 Department of Scalable Analysis and Visualization

So far we've experimented with varying the tolerance for clustering, while using start and end points, encircled area, and travel distance as features for North American flights.

Next, we will investigate additional combinations and explore additional features including turn angle, velocity, altitude, and perimeter, to determine anomalous trajectories.

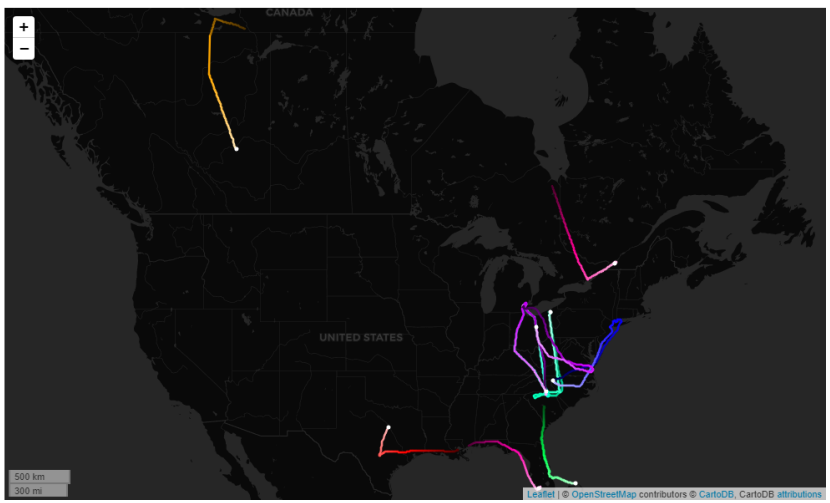

Figure 1. High amount of encircled area with low travel distance

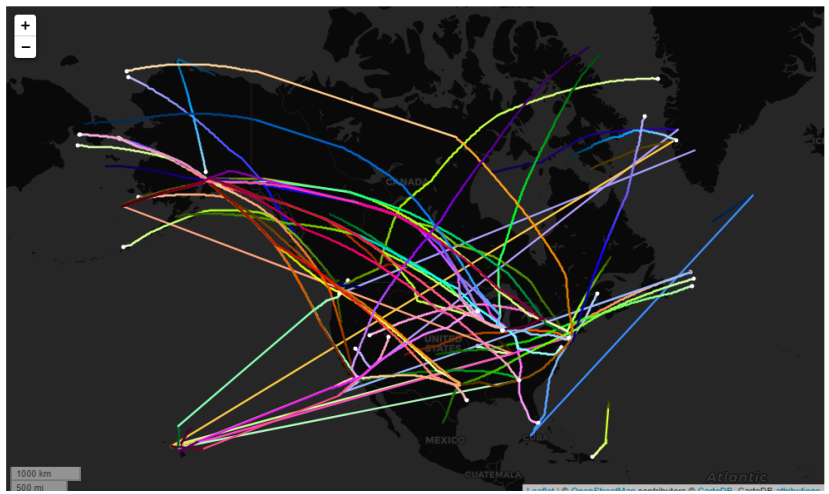

Figure 2. Outliers from clustering by start and end point locations

SAND2021-8778 PE

Implementation of Recovery discontinuous Galerkin algorithm in EMPIRE

CSRI Summer Proceedings 2021

Presented by: Megan McCracken

SAND2021-8736 A

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Implementation of Recovery discontinuous Galerkin algorithm in EMPIRE

Intern: Megan McCracken, Virginia Tech, **Virtual at:** Blacksburg, VA
Mentor: Sean Miller, 1446 Department of Computer Science

Abstract The recovery discontinuous Galerkin method recovers a smooth local solution that would be considered weakly equal to the discrete discontinuous solution of the diffusive flux terms. This method can be applied to both structured and unstructured grids and is used to resolve the smooth solution between the union of two cells. This project focuses on the implementation of a recovery algorithm for the diffusive fluxes seen in the Navier-Stokes equation set, as well as the application of RDG in EMPIRE for the relevant viscous terms. Tests on the achieved accuracy, stability, and speed will be conducted to see improvements made over previous calculation methods.

Problem Domain

Discontinuous Galerkin integration

Technical Approach

Recovery algorithm

Mission Application

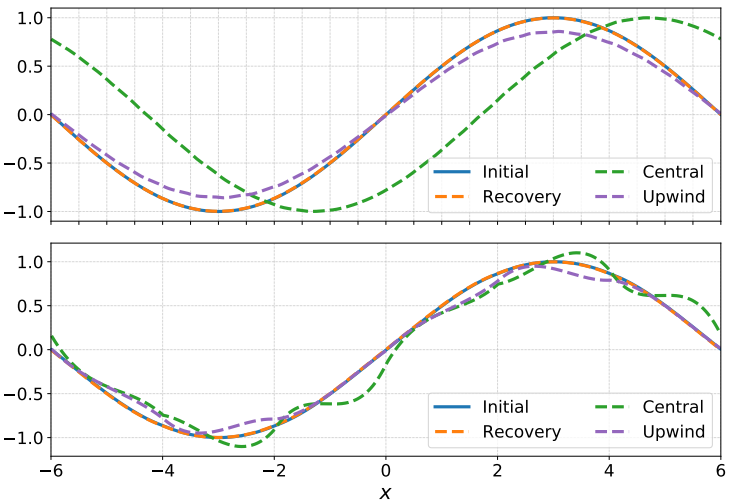
Algorithm development

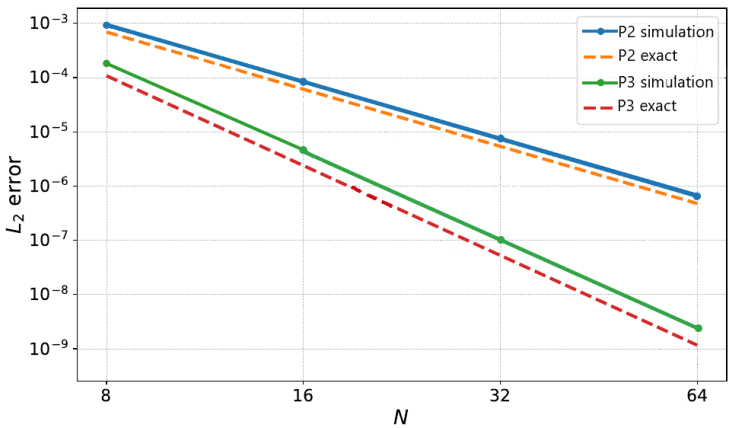
SAND2021-8736 A

Implementation of Recovery discontinuous Galerkin algorithm in EMPIRE : preliminary results

Intern: Megan McCracken, Virginia Tech, **Virtual at:** Blacksburg, VA
Mentor: Sean Miller, 1446 Department of Computer Science

Below are the some preliminary results created from the prototype recovery algorithm.





SAND2021-8736 A

Integrating PGAS and MPI-Based Graph Analysis

CSRI Summer Proceedings 2021

Presented by: Trevor McCrary

SAND2021-8810 D

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Integrating PGAS and MPI-Based Graph Analysis

Intern: Trevor McCrary, Mississippi State University, **Virtual at:** Starkville, Mississippi
Mentor: Karen Devine, 1465 Department of Scalable Algorithms

Abstract This project demonstrates that Chapel programs can interface with MPI-based libraries written in C++ **without storing multiple copies of shared data**. Chapel is a language for productive parallel computing using global namespaces (PGAS). We identified two approaches to interface Chapel code with the MPI-based Grafiki and Trilinos libraries. The first uses a single Chapel executable to call a C function that interacts with the C++ libraries. The second uses the mmap function to allow separate executables to read and write to the same block of memory on a node.

Problem Domain

Graph Analysis

Technical Approach

PGAS + MPI

Mission Application

Strategic Partnerships

SAND2021-8810 D

Integrating PGAS and MPI-Based Graph Analysis preliminary results

Intern: Trevor McCrary, Mississippi State University, **Virtual at:** Starkville, Mississippi
Mentor: Karen Devine, 1465 Department of Scalable Algorithms

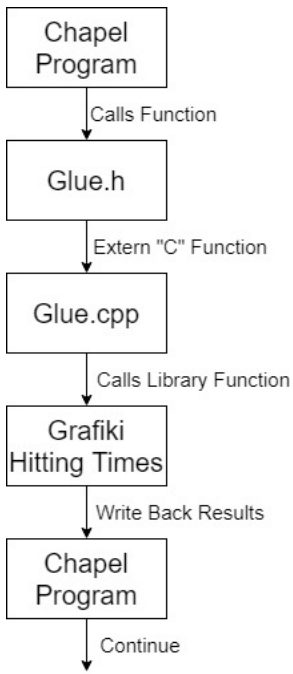

Figure: Method 1: a single Chapel executable calls a C function that interacts with the C++ libraries

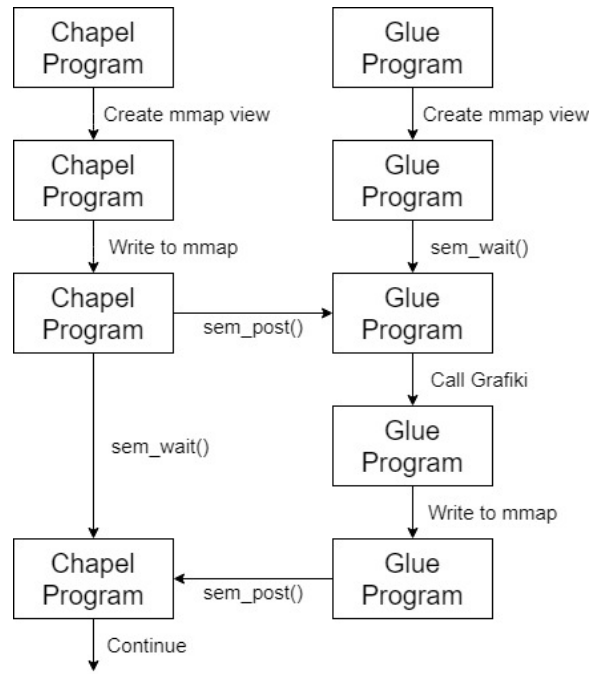

Figure: Method 2: two executables use the mmap function to read and write to the same block of memory.

SAND2021-8810 D

Goal-oriented data-driven reduced-order modeling guided by hyper-differential sensitivity analysis

Shane McQuarrie, University of Texas at Austin
Bart van Bloemen Waanders, 01463 (Optimization and UQ)
SAND2021-8586 D

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Goal-oriented data-driven reduced-order modeling guided by hyper-differential sensitivity analysis

Intern: Shane McQuarrie, University of Texas at Austin, **Virtual at:** Austin, Texas
Mentor: Bart van Bloemen Waanders, 01463 (Optimization and UQ)

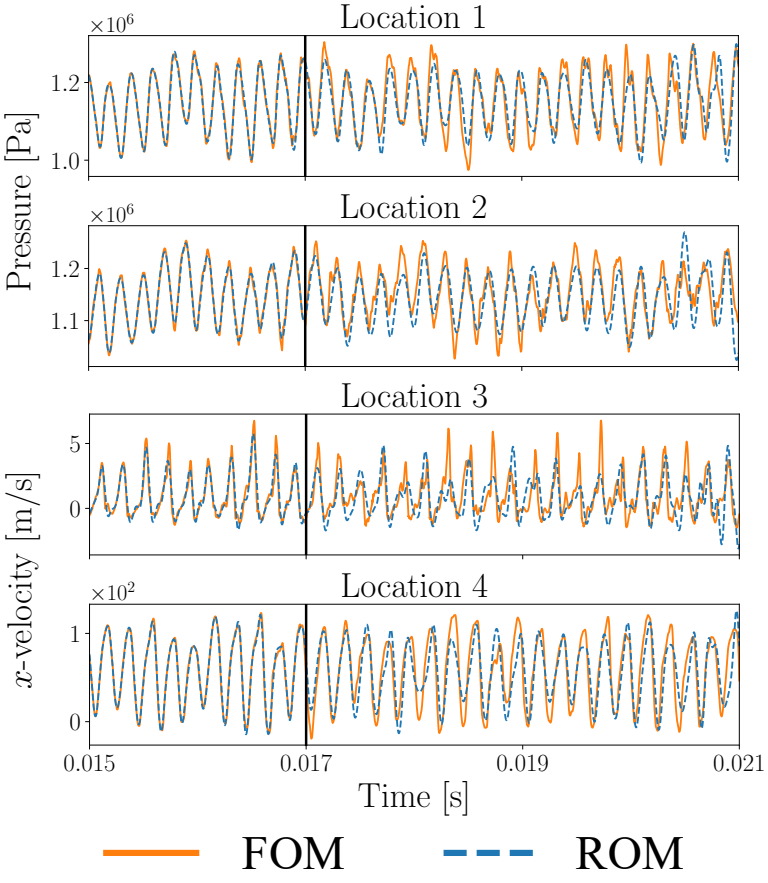
Abstract Harnessing the power of physics-based models for decision making is challenging but critical in many engineering analyses. Accordingly, surrogate models with reduced computational complexity are necessary to combat the prohibitive costs of high-fidelity simulations. Operator Inference (OpInf) has recently emerged as a data-driven paradigm of constructing physics-based reduced-order models. To guide the effectiveness of OpInf in the context of decision making, we leverage hyper-differential sensitivity analysis (HDSA) to determine the influence of the model form error on the solution of a relevant optimization problem. These specialized sensitivities are then used to direct the OpInf procedure to improve the quality of the reduced-order model in a goal-oriented fashion.

Problem Domain	**Technical Approach**	**Mission Application**
Reduced-order Modeling	OpInf, HDSA	Reactive Flows

Goal-oriented data-driven reduced-order modeling guided by hyper-differential sensitivity analysis

Intern: Shane McQuarrie, University of Texas at Austin, **Virtual at:** Austin, Texas
Mentor: Bart van Bloemen Waanders, 01463 (Optimization and UQ)

Sample results



Next steps

- Instrument HDSA for model form error associated with OpInf reduced-order models
- Relate the HDSA sensitivities to training data to add to the OpInf learning procedure
- Demonstrate the guided learning pipeline on problems of increasing complexity

Comparing Intel Compilers

CSRI Summer Proceedings 2021

Presented by: Nicholas Miller

SAND2021-8661 D

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[Comparing Intel Compilers]

Intern: Nicholas Miller, University of Central Florida
Virtual at: Orlando, Florida
Mentor: Clayton Hughes, Department of Scalable Computer Architecture (01422)

Abstract Intel recently released a new toolchain called oneAPI, which is shipped with a new LLVM-based compiler. This represents a significant change from its legacy compiler, which has been used extensively throughout the DOE. The upcoming Crossroads supercomputer will feature Intel Sapphire Rapids processors, making it critical to understand and document differences between the two compilers. This work will use a series of proxy applications to quantify the performance differences between the compilers and isolate the root cause of any significant changes in application behavior.

Problem Domain

Computer Performance

Technical Approach

Isolate Performance Using Low-Level Tools

Mission Application

Nuclear Deterrence (ND)

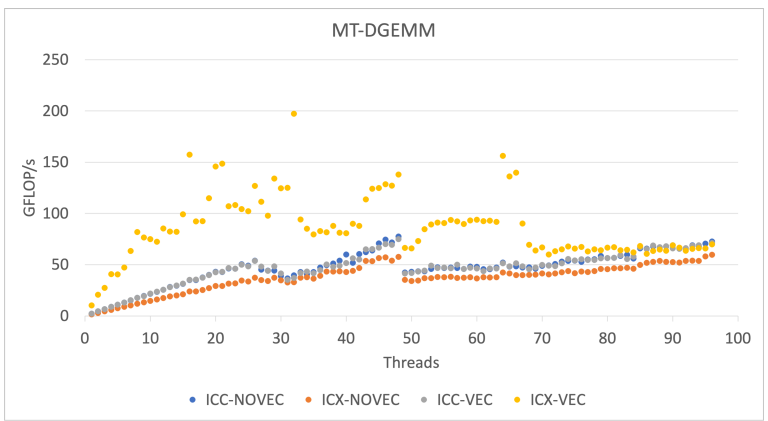
SAND2021-8661 D

Early Results

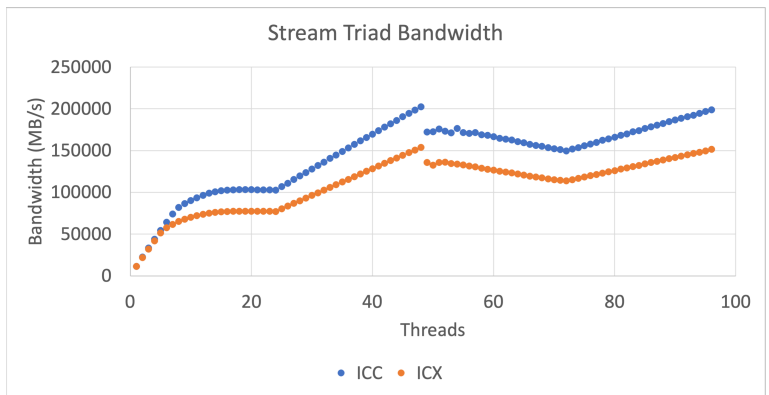
Sandia National Laboratories

Intern: Nicholas Miller, University of Central Florida
Virtual at: Orlando, Florida
Mentor: Clayton Hughes, Department of Scalable Computer Architecture (01422)

Early experiments have shown that there is a difference in performance between the two compilers in certain workloads, as shown below.



The next step is to use the profiling tools available on the testbeds to root-cause the performance differences.



SAND2021-8661 D

Learning Algebraic Multigrid Prolongation with Residual Graph Neural Networks

CSRI Summer Proceedings 2021

Presented by: Nicholas Moore

SAND2021-8648D

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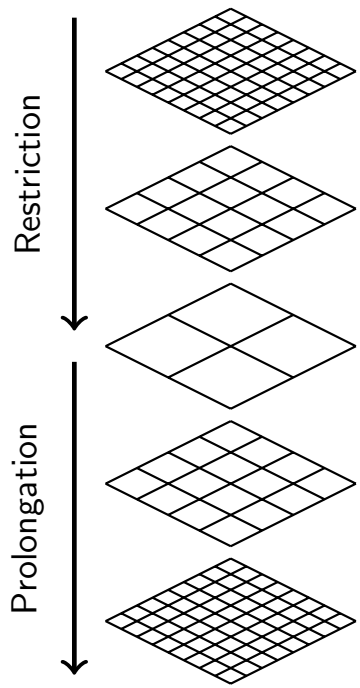
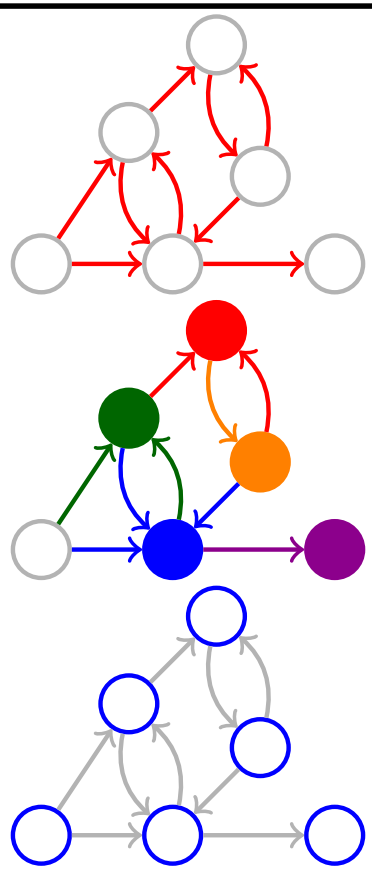
Learning Algebraic Multigrid Prolongation with Residual Graph Neural Networks

Intern: Nicholas Moore, Texas Tech University, **Virtual at:** Lubbock, TX
Mentors: Eric Cyr, 1442 Department of Computational Mathematics
Chris Siefert, 1465 Department of Scalable Algorithms

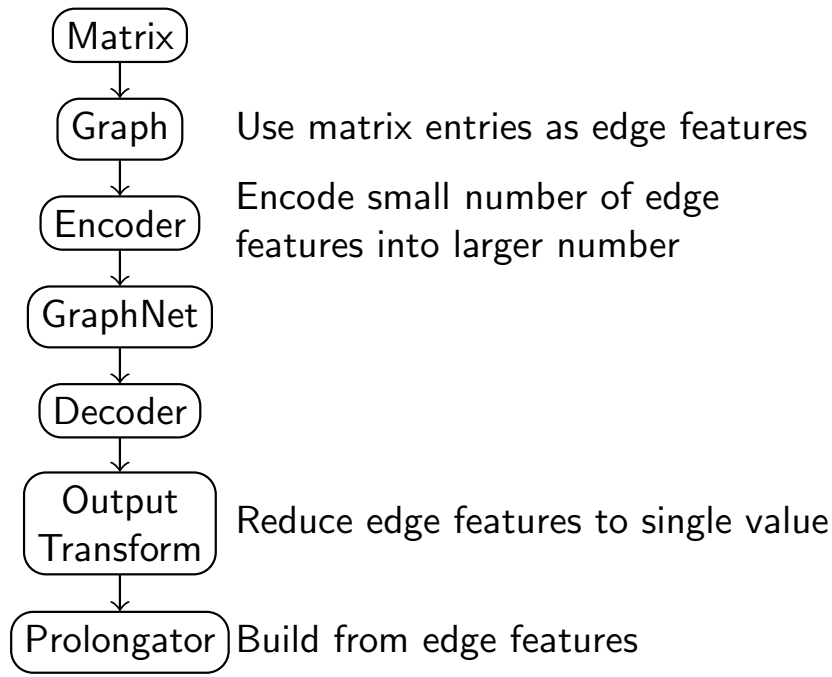
Multigrid



GraphNets



Matrix → Prolongation



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SAND2021-8648D

Comparison of Tempered and Truncated Fractional Models

CSRI Summer Proceedings 2021

Presented by: Hayley Olson

SAND2021-8692 C

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Comparison of Tempered and Truncated Fractional Models

Intern: Hayley Olson, University of Nebraska-Lincoln, **Virtual at:** Lincoln, Nebraska
Mentor: Marta D'Elia, 8754 Department of Quantitative Modeling & Analysis
Joint work with D'Elia and Gulian supported by DOE ASCR project PhILMs.

Abstract Consider the Fractional Laplace operator

$$\mathcal{L}_{frac}u(x) = \int_{\mathbb{R}^n} (u(x) - u(y))|x-y|^{-(n+2s)}\gamma_i(x,y)dy \tag{1}$$

where, for the tempered and truncated kernels we have

$$\gamma_{tem}(x,y;\lambda) = e^{-\lambda|x-y|} \qquad \gamma_{tr}(x,y;\delta,\sigma) = \sigma(x)\,\chi\{|x-y| < \delta(x)\}. \tag{2}$$

We train parameters $\delta(x)$ and $\sigma(x)$ in order to minimize the difference of the action of the operators over a set of test functions $\{u_i\}_{i=1}^N$; in particular, we minimize

$$\text{Loss}(\delta,\sigma) = \sum_{i=1}^{N} \|\mathcal{L}_{tem}u_i(x) - \mathcal{L}_{tr}u_i(x)\|_{L^2(\Omega)}, \quad \text{for } \Omega \subset \mathbb{R}^n.$$

The goal is to be able to replace the tempered fractional Laplacian with the computationally less intensive truncated fractional Laplacian.

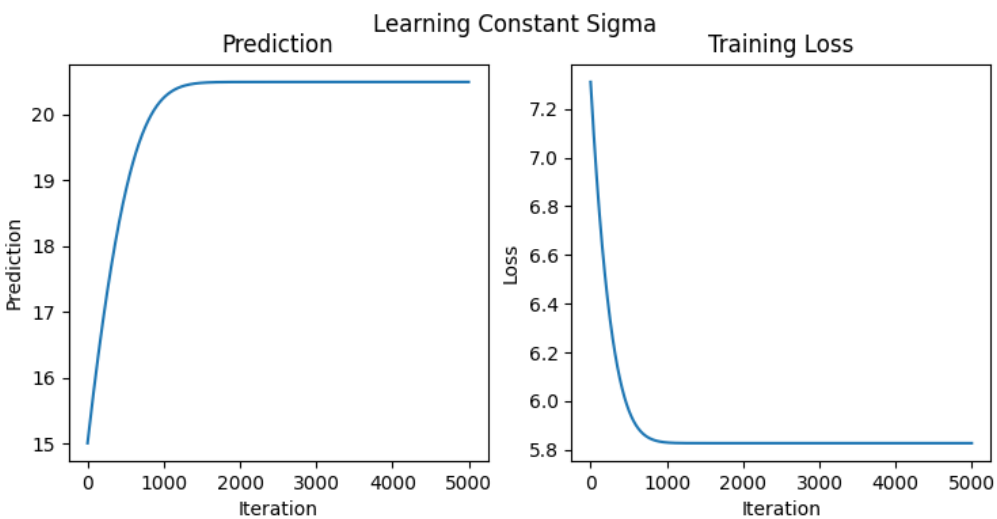
Problem Domain	**Technical Approach**	**Mission Application**
Fractional Order Operators	Nonlocal Vector Calculus & Machine Learning	Subsurface Transport & Turbulence

SAND2021-8692 C

Comparison of Tempered and Truncated Fractional Models

Intern: Hayley Olson, University of Nebraska-Lincoln, **Virtual at:** Lincoln, Nebraska
Mentor: Marta D'Elia, 8754 Department of Quantitative Modeling & Analysis
Joint work with D'Elia and Gulian supported by DOE ASCR project PhILMs.

Our preliminary experiments have found a constant σ that minimizes the L^2 difference of the operators on a training set. **Note:** the error is relatively large $\rightarrow$ optimizing wrt δ should yield a lower loss.



We are developing scripts that can learn the following parameters:

- $\sigma(x)$
- $\delta(x)$
- $\sigma(x)$ and $\delta(x)$ simultaneously.

We expect the latter to yield low Loss values.

SAND2021-8692 C

Multifidelity data fusion in convolutional encoder/decoder assembly networks for computational fluid dynamics

CSRI Summer Proceedings 2021

Presented by: Lauren Partin

SAND2021-8539 C

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Multifidelity data fusion in convolutional encoder/decoder assembly networks for computational fluid dynamics

Intern: Lauren Partin, University of Notre Dame, **Virtual at:** South Bend, IN
Mentors: Gianluca Geraci, Ahmad Rushdi, Michael S. Eldred, 1463 Optimization and UQ

Abstract In order to investigate multifidelity training, we analyze the regression accuracy of convolutional neural networks assembled from encoders (E), decoders (D) and skip connections. These networks benefit from a significant reduction in the number of trainable parameters with respect to an equivalent fully connected network. These architectures are also versatile with respect to the dimensionality of the inputs and outputs. For example, ED, DE or DED architectures are well suited to learn mappings between input and outputs of any dimensionality. We demonstrate the accuracy produced by such architectures when trained on a few high-fidelity and many low-fidelity data generated from the numerical solution of partial differential equations. In addition to the efficient training via multifidelity data, these networks introduce the possibility to produce multifidelity surrogates to be used in approximate control variate schemes for uncertainty quantification. Specifically, we quantify predictive uncertainty using a dropblock regularizer.

Problem Domain	**Technical Approach**	**Mission Application**
Neural networks for UQ	Multifidelity training	Fluid dynamics

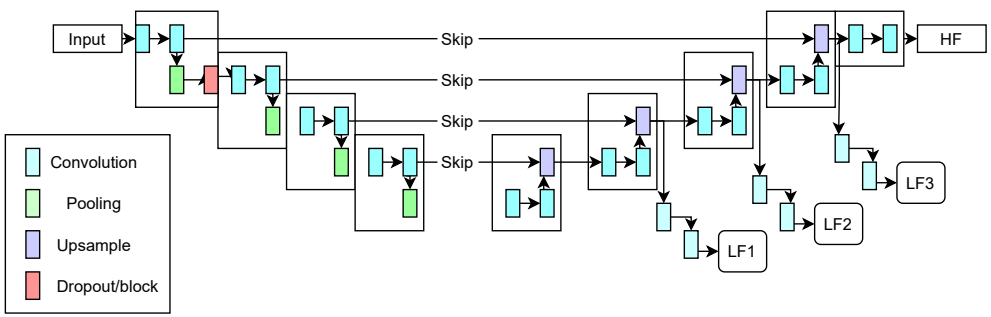
SAND2021-8539 C

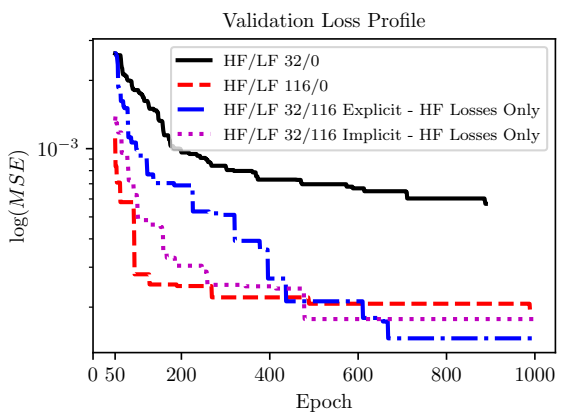
Multifidelity data fusion in convolutional encoder/decoder assembly networks for computational fluid dynamics preliminary results

Intern: Lauren Partin, University of Notre Dame, **Virtual at:** South Bend, IN
Mentors: Gianluca Geraci, Ahmad Rushdi, Michael S. Eldred, 1463 Optimization and UQ

Preliminary experiments show that our multifidelity convolutional network can use and generate multiple low resolution flow predictors to improve the accuracy of the flow at a higher resolution.

Next, we will investigate generalizations using combinations of low or high dimensional inputs/outputs using composable encoder-decoder architectures.





SAND2021-8539 C

Improved vertical remapping accuracy

CSRI Summer Proceedings 2021

Presented by: Jason Torchinsky

SAND2021-8711 PE

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This work describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Improved vertical remapping accuracy

Intern: Jason Torchinsky, University of Wisconsin-Madison, **Virtual at:** Madison, Wisconsin
Mentor: Mark Taylor, 1446 Department of Computational Science

Abstract A vertical Lagrangian coordinate has been used in global climate models for nearly two decades and has several advatanges over other discretizations, including reducing the dimensionality of the physical problem. As the Lagrangian surfaces deform over time, it is necessary to accurately and conservatively remap the vertical Lagrangian coordinate back to a fixed Eulerian coordinate. A popular choice of remapping algorithm is the piecewise parabolic method, a modified version of which is used in the atmospheric component of the Department of Energy's Energy Exascale Earth System Model. However, this version of the remapping algorithm creates unwanted noise at the model top and planetary surface. We describe the issues with this version of the algorithm and introduce a modification which eleminates this noise for several test cases.

Problem Domain

Remapping algorithms

Technical Approach

Piecewise parabolic method

Mission Application

Geosciences

SAND2021-8711 PE

Improved vertical remapping accuracy preliminary results

Intern: Jason Torchinsky, University of Wisconsin-Madison, **Virtual at:** Madison, Wisconsin
Mentor: Mark Taylor, 1446 Department of Computational Science

Our preliminary experiments have shown that the primary cause of the noise is the error introduced by requirement of local-bounds preservation at the domain boundary.

Next, we will investigate changes to the remapping algorithm to minimize the propagation of this error into the interior of the domain.

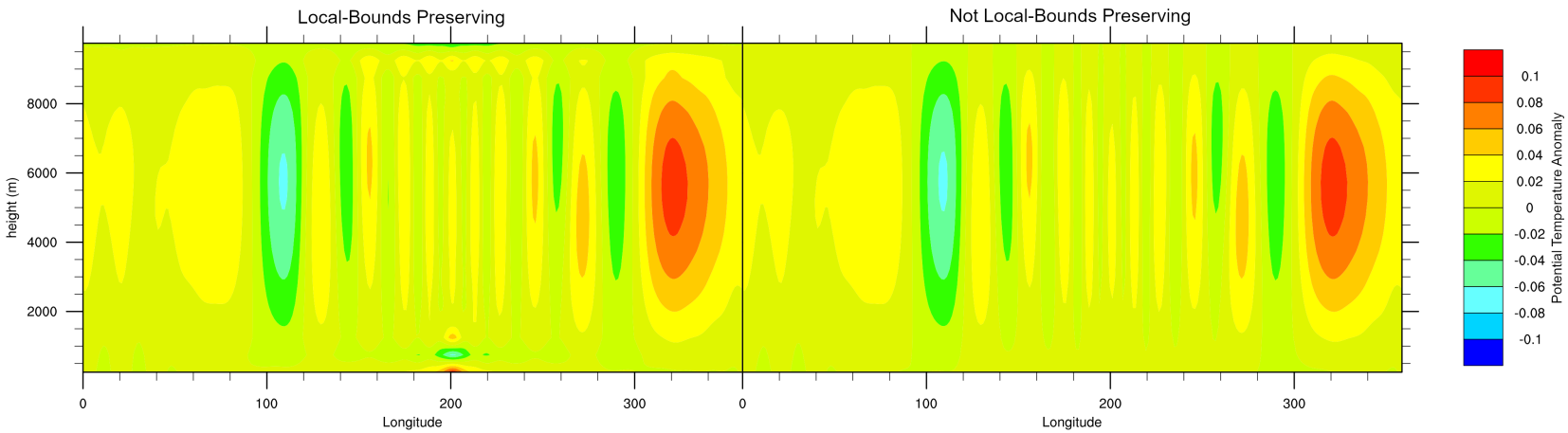

Figure: Longtiude-height cross-section of the potenital temperature anomaly at the equator for a standard non-hydrostatic gravity wave test case.

SAND2021-8711 PE

Sensitivity Analysis and Model Reduction in Plasma Dynamical Systems

CSRI Summer Proceedings 2021

Presented by: Ryan Chen

SAND2021-8756 D

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Sensitivity Analysis and Model Reduction in Plasma Dynamical Systems

Intern: Ryan Chen, United States Air Force Academy, **Hybrid at:** Livermore, CA
Mentor: Tiernan Casey, 8759 - Extreme scale data science and analytics

Abstract During atmospheric reentry at hypersonic speeds, air near the vehicle surface becomes superheated to the point where a plasma sheath is formed. In this chemical systems, thousands of reactions including ionization, dissociation, and vibrational excitation cause the number density of species to evolve over time. As a consequence, investigating quantities of interest in this environment through direct numerical simulation becomes very computationally expensive. In this project, a 7621 reaction plasma dynamical system was reduced in dimensionality while maintaining a low prediction error for two quantities of interest: vibrational energy and charge density. The model reduction was broken into initial physics intuition and sensitivity analysis stages. Finally, computationally efficient low dimensional surrogate models were trained for each quantity of interest and compared with the full model.

Problem Domain

Plasma Chemistry

Technical Approach

Surrogate Modeling

Mission Application

Hypersonics

SAND2021-8756 D

A reduced space simultaneous approach for optimization of nonlinear index-1 differential algebraic equations

CSRI Summer Proceedings 2021

Presented by: Robert Parker

SAND2021-8859 D

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A reduced space simultaneous approach for optimization of nonlinear index-1 differential algebraic equations

Intern: Robert Parker, Carnegie Mellon University, **Virtual at:** Pittsburgh, PA
Mentor: Bethany Nicholson, 1464 Discrete Math and Optimization

Abstract Power generation equipment such as boilers, reactors, and adsorbers may be described by systems of nonlinear differential and algebraic equations (DAEs). A common approach for optimization of these systems is to include the fully discretized equations in a nonlinear program (NLP) as equality constraints. These problems can be difficult to converge if algebraic equations are poorly scaled. We propose an NLP formulation for index-1 DAEs in which algebraic equations are removed from the optimization problem and replaced with equivalent implicit functions. These implicit functions admit exact first and second derivatives via the implicit function theorem, allowing the NLP algorithm to maintain its convergence properties. Furthermore, the algebraic subsystem may decompose via block triangularization, improving the speed and reliability of the implicit function evaluation.

Problem Domain	**Technical Approach**	**Mission Application**
Dynamic optimization	Implicit functions	Power generation

SAND2021-8859 D

Prototype implementation is completed; trials are underway

Intern: Robert Parker, Carnegie Mellon University, **Virtual at:** Pittsburgh, PA
Mentor: Bethany Nicholson, 1464 Discrete Math and Optimization

A semi-explicit index-1 DAE has the form:

$$\begin{aligned} \dot{x} &= f(x, y, u) \\ 0 &= g(x, y, u), \ \det(\nabla_y g) \neq 0 \end{aligned} \tag{1}$$

Our implicit function implementation handles systems:

$$\begin{aligned} F(z, y) &= 0 \\ G(z, y) &= 0, \ \dim(G) = \dim(y) \end{aligned} \tag{2}$$

First and second derivatives are via the implicit function theorem:

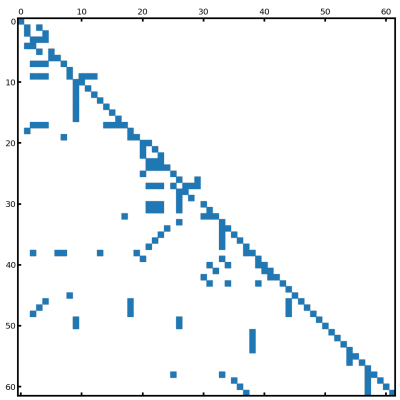
$$\nabla_z y = -\nabla_y G^{-1} \nabla_z G$$

$$\nabla^2_{zz} y = -\nabla_y G^{-1} \left(\nabla^2_{zz} G + \left(\nabla^2_{zy} G^T \nabla_z y + \nabla_z y^T \nabla^2_{zy} G \right) + \nabla_z y^T \nabla^2_{yy} G \nabla_z y \right) \tag{3}$$

Application: Chemical looping combustion (CLC) reactor
Algebraic equations are:

- Highly nonlinear
- Highly decomposable

Figure: Algebraic Jacobian, $\nabla_y g$, of CLC reactor model



SAND2021-8859 D