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Scalable High-order Methods for Multi-Scale Problems Analysis, Algorithms, and Applications

Mark Ainsworth
BROWN UNIVERSITY IN PROVIDENCE IN STATE OF RI AND PROVIDENCE PLANTATIONS

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Final Report

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14. ABSTRACT

It is anticipated that in future generations of massively parallel computer systems a significant portion of processors may suffer from hardware or software faults rendering large-scale computations useless. In this project, the PI and his students address this problem from the algorithmic side, proposing resilient frameworks that can recover and continue the solution with gappy fields from such faults irrespective of their fault origin. In addition to its robustness and resilience, the new framework generalizes previous multiscale and multifidelity approaches in a unified parallel computational framework.

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FINAL REPORT: Scalable High-order Methods for Multi-scale Problems: Analysis, Algorithms and Applications
AFOSR Grant Number:FA9550-12-1-0463

George Em Karniadakis

Division of Applied Mathematics
Brown University

Abstract

It is anticipated that in future generations of massively parallel computer systems a significant portion of processors may suffer from hardware or software faults rendering large-scale computations useless. In this project, the PI and his students address this problem from the algorithmic side, proposing resilient frameworks that can recover and continue the solution with gappy fields from such faults irrespective of their fault origin. In addition to its robustness and resilience, the new framework generalizes previous multiscale and multifidelity approaches in a unified parallel computational framework.

Objectives

The general objective of this project was to develop a general CFD framework for multifidelity simulations to target multiscale problems but also resilience in exascale simulations. The specific objective was to develop a fault-recovery and fault-resilient algorithm using approximation theory, domain decomposition, and machine learning based information-fusion together.

Approach

Fault-recovery algorithm

We employ three different types of recovery algorithms, namely (1) projective integration (temporal estimation), (2) coKriging (spatial estimation), and (3) resimulation (spatio-temporal estimation). We introduce the concepts of the three approaches briefly next, for detail see (S. Lee et al. 2015).

First, if numerical solutions are sufficiently smooth in time, the temporal estimation based on previous saved data can give a highly accurate result on a missing part of the solution. To accomplish this, we employ an equation-free/Galerkin-free projective integration. The projective integration is based on the proper orthogonal decomposition (POD) for a dimension reduction. The basic algorithm of the projective integration consists of three stages: the restriction (a dimension reduction by POD), estimation (of the coefficient for the POD basis), and lifting (a reconstruction of the gappy field).

While for the temporal estimation we use the previous flow field data and smoothness in time, in the spatial estimation we need to use geometrically neighboring data points at the current time to exploit smoothness in space. In this project, a "multi-fidelity coKriging interpolation method", the unbiased linear interpolation, is introduced for estimating the missing part.

The "resimulation" method is employed to solve the Navier-Stokes equations again on the missing part only with estimated initial condition (by the coKriging) and estimated field variables at the boundary (by the projective integration), see Figure 1.

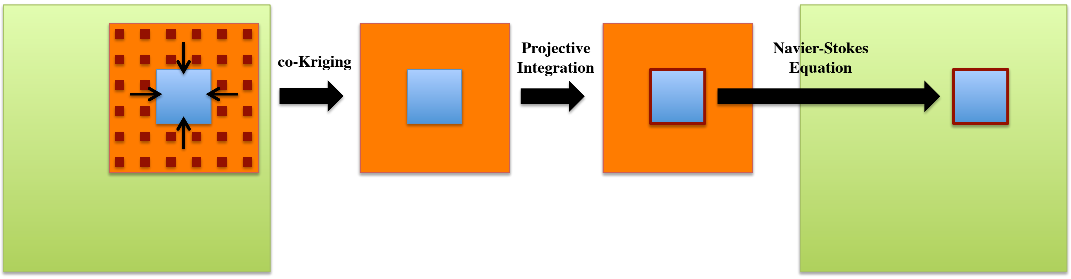


Figure 1: "Re-simulation" with estimated boundary condition: First, we estimate the initial condition for the missing part (blue) with two sample sets: refined (orange) and coarse (red). Subsequently, we use the projective integration to update the boundary using the refined sample set. Finally, we solve the Navier-Stokes equation in the missing part only.

Fault-resilient algorithm – Gappy simulation

In the gappy simulation framework, we compute explicitly the solution to a PDE not on the entire domain but only partially on some sub-domains with some auxiliary data that span the entire domain and obtained independently. The main idea is to combine the global coarse information with some finely resolved sub-domains and appropriately combine the two solutions to obtain a more accurate solution on the entire domain. This set up admits two different interpretations. From the multiscale perspective, the global coarse solution represents the large scales whereas the fine-resolution sub-domains represent regions of finer scales. The gappy regions may also be regions of finer scales but with spatial correlations determined by the resolved regions. From the parallel computing perspective, the gappy sub-domains may be regions corrupted by random software or hardware faults whereas the global coarse solution is obtained on an independent small set of processors, which is assumed to be immune to such faults that the big computer system may suffer from.

A flow chart of the gappy simulation is shown in Figure 2. First, upon notification of a fault detection (not discussed here), we check which domains are affected by errors, and define computational subdomains and gaps, respectively. Next, we choose a proper buffer size, and the gappy simulation estimates the fields at the local boundaries of each subdomain by the information fusion method using also the independent auxiliary data. After setting-up all the parameters and variables, the gappy simulation solves each subdomains on independent nodes during non-interaction time steps τ. After time τ, all subdomains are re-joined together and the buffer region of each subdomain is cut-off. Finally, using the auxiliary data, the new field variables at the boundaries can be updated via coKriging. The gappy simulation repeats again this procedure until the main simulation ends or all faults are fixed.

Main Results

The first main algorithmic result of this project is the reconstruction of missing data using three different approaches according to three fault scenarios. These lead to a robust and effective recovered solution in various fault scenarios. We have also developed the fault-resilient CFD algorithm in a unified parallel computational framework. Combining approximation theory and domain decomposition together with machine learning techniques, this results in robustness and resilience with low-resolution auxiliary data. We highlight some of the simulation results next.

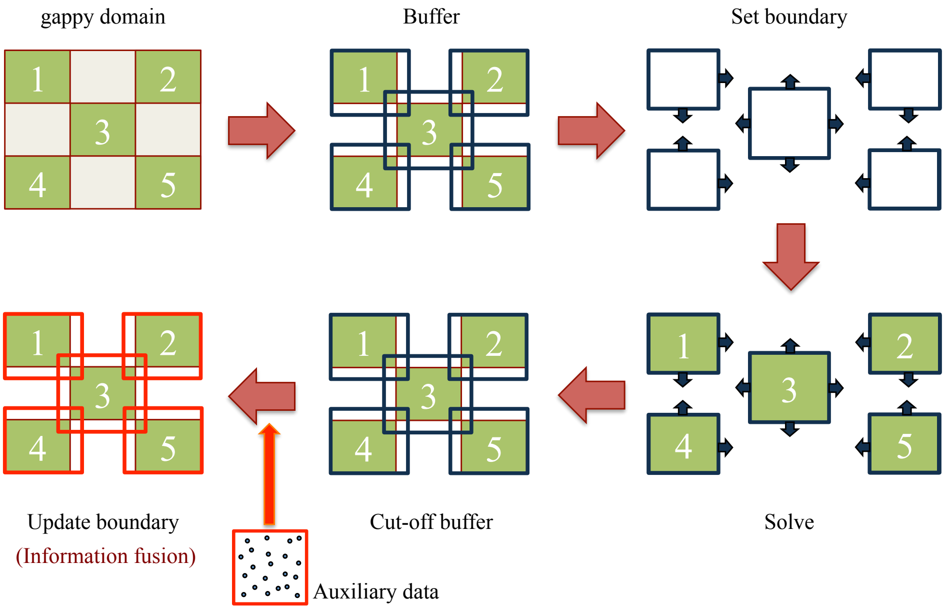


Figure 2: A flow chart for a gappy simulation (start from left-top): We first check where the gappy domains are located. Next, we choose a buffer size and estimate field variables at local boundaries. Each sub-domain is solved in parallel and independently during non-interaction time τ. After τ, all gappy domains are re-joined together after cutting-off the buffer region. Finally, using information fusion method with auxiliary data, all field variables are updated at the local boundaries of the subdomains. This is one complete cycle of the gappy simulation algorithm.

Fault-recovery Simulations

We present results for two benchmark problems – a lid-driven cavity flow (quasi-steady) and a flow past a cylinder (quasi-periodic), for details see (Lee et al, 2015). To this end, we consider three types of available fault scenarios: (1) a gappy region but with no previous gaps and no contamination of surrounding simulation data, (2) a space-time gappy region but with full spatiotemporal information and no contamination, and (3) previous gaps with contamination of surrounding data. To recover from such faults, we employ different reconstruction and simulation methods, namely the projective integration, the co-Kriging interpolation, and the resimulation method. The results with respect to RMS error and capability are shown in Tables 1 and 2. We summarize here the main findings of our study:

- For sufficiently small time gaps, the projective integration method is the best while for longer time gaps the co-Kriging method is better.
- Overall, the "resimulation" method seems to be the most robust method, performing well in all three fault scenarios.
- Estimating the boundary condition using projective integration leads to accurate results for the "resimulation" method in scenario 3 where the other two methods fail.

Fault-resilient Simulations

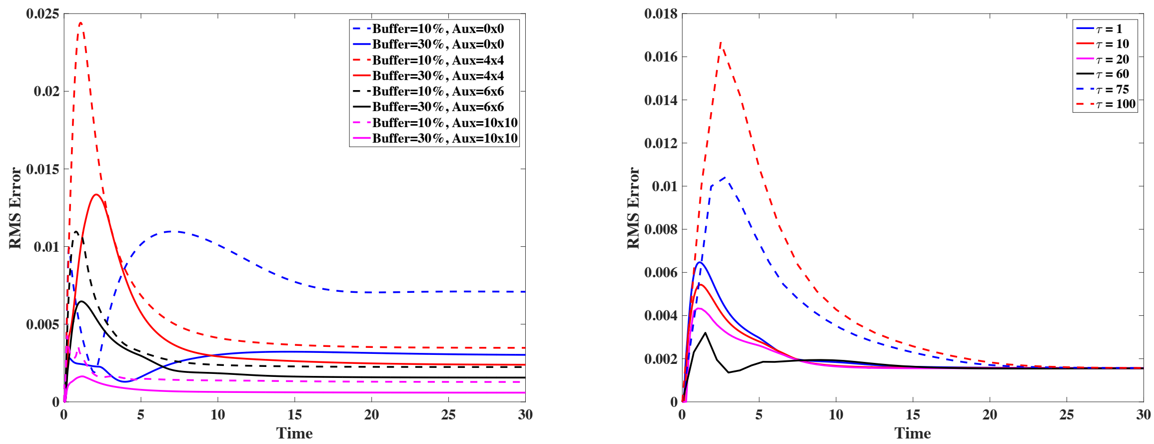
We apply our fault-resilient framework to the heat equation and the Navier-Stokes equations, and obtain important first results via a parametric study. Specifically, we employ the finite difference method to perform

Table 1: Comparison of RMS error for three different methods in lid-driven cavity flow. “–” represent inability for corresponding scenario.

Velocity	Time gaps (ΔT_g)	Scenario	P.I.	CoKriging	Resimulation
streamwise	0.5	1	0.0044	0.0136	0.0075
		2	—	0.0136	0.0074
		3	—	—	0.0078
	1.0	1	0.0156	0.0150	0.0124
		2	—	0.0150	0.0122
		3	—	—	0.0158
crossflow	0.5	1	0.0007	0.0177	0.0060
		2	—	0.0177	0.0059
		3	—	—	0.0088
	1.0	1	0.0116	0.0192	0.0108
		2	—	0.0192	0.0106
		3	—	—	0.0105

Table 2: Comparison of RMS error for three different methods in flow past a circular cylinder. “–” represent inability for corresponding scenario.

Velocity	Time gaps (ΔT_g)	Scenario	P.I.	CoKriging	Resimulation
streamwise	0.27	1	0.0039	0.0219	0.0060
		2	—	0.0219	0.0172
		3	—	—	0.0175
	0.47	1	0.0193	0.0251	0.0144
		2	—	0.0251	0.0235
		3	—	—	0.0291
crossflow	0.27	1	0.0046	0.0178	0.0065
		2	—	0.0178	0.0168
		3	—	—	0.0189
	0.47	1	0.0231	0.0159	0.0149
		2	—	0.0159	0.0241
		3	—	—	0.0374



(a) Buffer and Auxiliary data

(b) Non-interaction time (τ)

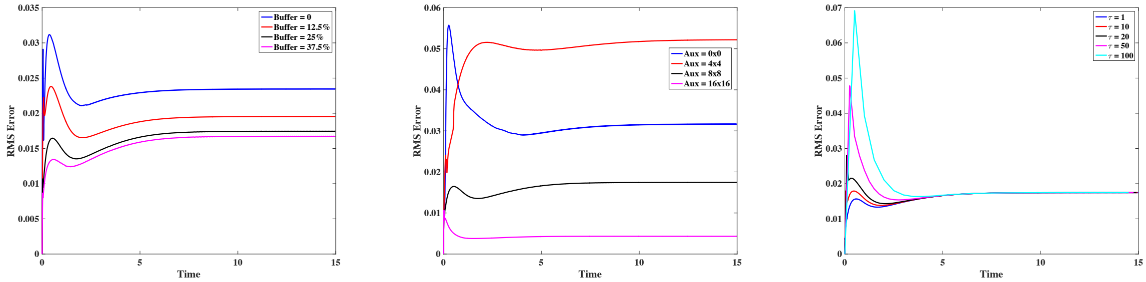
Figure 3: Time history of the RMS error in the heat equation with different parameters. In (a), a fixed parameters is τ=1. In (b), fixed parameters are the buffer=30% and the auxiliary data=6×6 grid.

a gappy simulation in both benchmark problems. The gappy domains looks like a checker board, see Figure 2. We observe that the RMS error of all test simulations are converging to zero at steady-state. Moreover, we investigate the key parameters of this framework: 1) type of correlation kernel, 2) size of buffer, 3) accuracy of auxiliary data, and 4) non-interaction time, τ. The results of our parametric study are shown in Figure 3 and 4. We summarize here the main findings of our study below:

- ***Kernel***: the Matérn kernel is found to be the best kernel with respect to RMS error and stability in both problems.
- ***Buffer***: the bigger buffer can guarantee the smaller RMS error in both problems because the error at the local boundary can be diffused in a buffer region. Moreover, as the auxiliary data is inaccurate or auxiliary data may not be available, the size of buffer enhances the effectiveness in this framework.
- ***Auxiliary data***: the finer resolution auxiliary data gives the smaller RMS error in both problems because of increasing accuracy of results by information fusion. As shown in Figure 3 and 4, the accuracy of auxiliary data is found to be the most important parameter to reduce the RMS error effectively.
- ***Non-interaction time (τ)***: In the heat equation (only diffusion), near the *allowable* τ, calculated by the estimation of a penetration length for a diffusion, we can guarantee the smaller RMS error. However, in the Navier-Stokes equations (combined diffusion and advection), the smaller τ (update boundary values more frequently) gives the smallest RMS error.

Acknowledgement/Disclaimer

This work was sponsored by the Air Force Office of Scientific Research, under grant/contract number FA9550-12-1-0463. The views and conclusions contained herein are those of the author and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.



(a) Buffer (b) Auxiliary data (c) Non-interaction time (τ)

Figure 4: Time history of the RMS error in a Naiver-Stokes equation with different parameters. In (a), fixed parameters are τ=5 and auxiliary data=8×8 grid. In (b), fixed parameters are the buffer = 25% and the τ=5. In (c) fixed parameters are the buffer=25% and the auxiliary data= 8×8 grid.

Personnel Supported During Duration of Grant

- Faculty: G. E. Karniadakis, The Charles Pitts Robinson and John Palmer Barstow Professor of Applied Mathematics, Brown University.
- PhD Student: Seungjoon Lee, Paris Perdikaris, Yu-Hang Tang, Brown University

Honors & Award

- Society for Industrial and Applied Mathematics, 2015, Ralph E Kleinman Award.
- US Association of Computational Mechanics, 2013, Tinsley Oden medal (inaugural)
- US Association of Computational Mechanics, 2007, Computational Fluid Dynamics award.
- Fellow of SIAM, 2011-.
- Fellow of the American Physical Society, 2004.
- Fellow of the American Society of Mechanical Engineers, 2003.
- Associate Editor of Journal of Computational Physics, 2005.

Publications

1. S. Lee, I.G. Kevrekidis and G.E. Karniadakis, "Resilient algorithms for reconstructing and simulating gappy flow fields in CFD", Fluid Dynamic Research, vol. 47, 051402, 2015.
2. Y. Yu, H. Yan, Y. Constantinidis, O. Oakley and G.E. Karniadakis, "Suppression of vortex-induced vibrations by fairings: A numerical study", Journal of Fluid Structures, vol. 54, 679-700, 2015.
3. Y. Yu, M. Bittencourt and G.E. Karniadakis, "A semi-local spectral/hp element solver for linear elasticity problems", International Journal for Numerical Methods in Engineering, vol. 10, 347-373, 2014.

Interactions/Transitions

The PI and his group had interaction with Prof. I.G. Kevrekidis (Princeton University) on issues related to the gappy simulations for the fault resilient algorithm and the projective integration method for the fault recovery approach.

1.

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Abstract

The first main algorithmic result of this project is the reconstruction of missing data using three different approaches according to three fault scenarios. These lead to a robust and effective recovered solution in various fault scenarios. We have also developed the fault-resilient CFD algorithm in a unified parallel computational framework. Combining approximation theory and domain decomposition together with machine
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