Final Technical Report

DOE Award Number: DE-SC0010540

Recipient: Duke University

Project Title: Probabilistic Approach to Enable Extreme-Scale Simulations under Uncertainty and System Faults

Principal Investigator: Omar M. Knio
Department of Mechanical Engineering and Materials Science
Duke University
144 Hudson Hall, Box 90300
Durham, NC 27708

Date: May 5, 2017

Project Goals

In order to resolve key processes in DOE mission-critical applications such as climate prediction or combustion simulation, the required computational resources are several orders of magnitude more powerful than the current state-of-the-art leadership computing facilities. As computing platforms evolve towards such extreme scales, scientific simulation codes will need to run effectively on millions of nodes and also take advantage of strong local concurrency through multiple cores or threads per node. Besides the need for extreme scalability, it is expected that such extreme scale computing platforms will generate many hard faults (e.g. nodes failing) and soft faults (e.g. silent data corruption due to random bit flips), thereby requiring scientific simulation codes to be robust against a wide variety of system faults. Besides the actual running of a scientific simulation on such extreme scale architectures, these challenges also have implications for the predictive fidelity of the associated simulation results. How does one account for the added uncertainty due to system faults, along with all other sources of uncertainty (e.g. uncertain input parameters and boundary conditions) that affect scientific simulations?

The current project develops a novel approach that uses a probabilistic description to capture the current state of knowledge about the computational solution. To effectively spread the computational effort over multiple nodes, the global computational domain is split into many subdomains. Computational uncertainty in the solution translates into uncertain boundary conditions for the equation system to be solved on those subdomains, and many independent, concurrent subdomain simulations are used to account for this boundary condition uncertainty. By relying on the fact that solutions on neighboring subdomains must agree with each other, a more accurate estimate for the global solution can be achieved. Statistical approaches in this update process make it possible to account for the effect of system faults in the probabilistic description of the computational solution, and the associated uncertainty is reduced through successive iterations. By combining all of these elements, the probabilistic reformulation allows splitting the computational work over very many independent tasks for good scalability, while being robust to system faults.

Accomplishments

We have developed a suite of resilient solvers for elliptic partial differential equations, all relying on a domain decomposition framework, in which the solution is sought as a probabilistic state of knowledge update.

Such reformulation allows resiliency with respect to potential faults without having to apply fault detection, avoids unnecessary communication, and is generally well-suited for rigorous uncertainty quantification studies that target improvements of predictive fidelity of scientific models.

Various algorithms belonging to this framework were developed and successfully tested within this project. These include:

1. algorithms based on either overlapping or non-overlapping domain decomposition techniques;

2. algorithms implementing non-separable elliptic PDEs in one and two-space dimensions;

3. algorithms for deterministic elliptic systems, and for elliptic systems with random diffusivity field.

In the resilient solution framework, parallel and independent solves of multiple deterministic local problems are used to define suitable representations of local boundary-to-boundary maps that are used to reconstruct the global solution. Various approaches have been developed and tested for this purpose, include solvers based on: (a) L1 and L2 approaches, (b) least absolute deviation, (c) lasso formulation, and (d) a hybrid LAD-lasso approach. n particular, computations with the hybrid approach have shown that the method can effectively overcome the occurrence of system faults.

In addition, we have also explored the possibility of enhancing the performance of resilient solvers by exploiting a priori bounds for the discrete solution. To this end, explicit bounds have been derived that reflect two contributions. First, the influence of boundary conditions is taken into account through a discrete maximum principle. Second, the contribution of the source field is evaluated in a fashion similar to that used in the treatment of the continuous a priori operators. Closed form expressions were, in particular, obtained for the case of a conservative, second-order finite difference approximation of the diffusion equation with variable scalar diffusivity. We have also demonstrated that the bounds are able to detect most system faults, and thus considerably enhance the resilience and the overall performance of our resilient solvers.

In collaborative work with the SNL team, we have contributed to the development of the Rexsss software framework. Rexsss incorporates:

1. domain decomposition techniques for deterministic and stochastic elliptic PDEs;

2. resilient solvers and preconditioners; and,

3. parallel implementations based on a single program multiple data (SPMD) model based on a one-to-one mapping between subdomain and MPI processes responsible for both state and computation; and (b) an asynchronous server-client implementation where all state information is held by the servers and clients are designed solely as computational units.

The capabilities afforded by this software framework have in particular enabled us to perform both resilience analysis and scalability assessment.

The fundamental, algorithmic, and software developments highlighted above have been documented in several journal publications [J1-J5], refereed conference proceedings [C1-C5], and a technical report [R1]. They have also been the subjected of lectures and presentations [L1-L18].

Publications/Presentations

Journal Publications:

J1 Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O.P. Le Maître, O.M. Knio, B.J. Debusschere (2017) "Exploring the Interplay of Resilience and Energy Consumption for a Task-Based Partial Differential Equations Preconditioner," submitted to *Parallel Computing*.

J2 P. Mycek, A. Contreras, O. Le Maître, K. Sargsyan, F. Rizzi, K. Morris, C. Safta, B. Debusschere, O. Knio (2017) "A Resilient Domain Decomposition Polynomial Chaos Solver for Uncertain Elliptic PDEs," *Computer Physics Communications* **216**, 18?34.

J3 F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O.P. Le Maître, O.M. Knio, B.J. Debusschere (2017) "Partial Differential Equations Preconditioner Resilient to Soft and Hard Faults," *International Journal of High Performance Computing Applications*, doi=10.1177/1094342016684975.

J4 P. Mycek, F. Rizzi, O. Le Maître, K. Sargsyan, K. Morris, C. Safta, B. Debusschere, O. Knio (2017) "Discrete a priori bounds for the detection of corrupted PDE solutions in exascale computations," *SIAM J. Sci. Comput.* **39**, C1-C28.

J5 K. Sargsyan, F. Rizzi, P. Mycek, C. Safta, K. Morris, H. Najm, O. Le Maître, O. Knio, B. Debusschere (2015) "Fault Resilient Domain Decomposition Preconditioner for PDEs," *SIAM Journal on Scientific Computing* **37**, A2317-A2345.

Refereed Conference Proceedings:

C1 K. Morris, F. Rizzi, B. Cook, P. Mycek, O. Le Maître, O.M. Knio, K. Sargsyan, K. Dahlgren, B.J. Debusschere (2016) "Performance Scaling Variability and Energy Analysis for a Resilient ULFM-based PDE Solver," Proceedings of 7th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems, Salt Lake City, UT, Nov 13, 2016.

C2 F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, Olivier Le Maître, O. Knio, B. Debusschere (2016) "ULFM-MPI Implementation of a Resilient Task-Based Partial Differential Equations Preconditioner," 6th Workshop on Fault-Tolerance for HPC at eXtreme Scale (FTXS 2016), at The 25th International ACM Symposium on High Performance Distributed Computing (HPDC 2016) Kyoto, Japan on May 31 - June 4, 2016.

C3 K. Morris, F. Rizzi, K. Sargsyan, K. Dahlgren, P. Mycek, C. Safta, O. Le Maître, O.M. Knio, and B.J. Debusschere (2016) "Scalability of Partial Differential Equations Preconditioner Resilient to Soft and Hard Faults," ISC High Performance, Frankfurt, Germany, Jun 19-23, 2016.

C4 F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. Le Maître, O.M. Knio, B.J. Debusschere (2016) aaExploring the Interplay of Resilience and Energy Consumption for a Task-Based Partial Differential Equations Preconditioner," PP4REE 2016 - Workshop on Parallel Programming for Resilience and Energy Efficiency at the Principles and Practice of Parallel Programming 2016 (PPOPP16) conference, Barcelona, Spain, March 12-16, 2016.

C5 F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. Le Maître, O. Knio, B. Debusschere "Partial Differential Equations Preconditioner Resilient to Soft and Hard Faults," 2015 IEEE International Conference on Cluster Computing (CLUSTER).

Reports:

R1 K. Sargsyan, F. Rizzi, P. Mycek, C. Safta, K. Morris, H. N. Najm, O. Le Maître, O. Knio, B. Debusschere (2015) "Fault Resilient Domain Decomposition Preconditioner for PDEs," SAND2015-4706.

Other Publications Acknowledging DOE Support:

O1 A.A. Contreras (2017) *Model Reduction and Domain Decomposition Methods for Uncertainty Quantification*, Ph.D. Thesis, Duke University.

O2 A.A. Contreras, P. Mycek, O.P. Le Maître, F. Rizzi, B. Debusschere, O.M. Knio (2017) "Parallel Domain Decomposition Strategies for Stochastic Elliptic Equations, Part A: Local KL Representations," in preparation for submission to *SIAM J. Sci. Comput.*

O3 A.A. Contreras, P. Mycek, O.P. Le Maître, F. Rizzi, B. Debusschere, O.M. Knio (2017) "Parallel Domain Decomposition Strategies for Stochastic Elliptic Equations, Part B: Accelerated Monte-Carlo Sampling with Local PC Expansions," in preparation for submission to *SIAM J. Sci. Comput.*

Lectures and Presentations

L1 P. Mycek, F. Rizzi, O. Le Maître, K. Sargsyan, K. Morris, C. Safta, B. Debusschere, O. Knio (2017) "Resilience Enhancement Using Discrete A Priori Bounds for the Detection of Faulty PDE Solutions," PASC17 Conference, Lugano, Switzerland, June 26-28.

L2 F. Rizzi, K. Morris, B. Cook, P. Mycek, O. Le Maître, O. Knio, K. Sargsyan, K. Dahlgren, B. Debusschere (2017) "Scaling and Energy Analysis for a Resilient ULFM-based PDE Solver," PASC17 Conference, Lugano, Switzerland, June 26-28.

L3 K. Morris, F. Rizzi, P. Mycek, O. Le Maître, O.M. Knio, A. Contreras, K. Sargsyan, C. Safta, B.J. Debusschere, (2017) "A Resilient Solver for 2D Uncertain Elliptic PDEs Via Fault-Tolerant MPI Server-Client-Based Implementation," presented at SIAM Conference on Computational Science and Engineering, Atlanta, GA, February 27 – March 3.

L4 F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, A. Contreras, C. Safta, O. Le Maître, O.M. Knio, B.J. Debusschere (2017) "Partial Differential Equations Solver Resilient to Soft and Hard Faults," presented at SIAM Conference on Computational Science and Engineering, Atlanta, GA, February 27 – March 3.

L5 A. Contreras, P. Mycek, O. Le Maître, F. Rizzi, K. Morris, K. Sargsyan, C. Safta, B.J. Debusschere, O.M. Knio (2017) "Acceleration of Monte Carlo Methods for Stochastic Elliptic PDEs Using Domain Decomposition and PC Approximations of Local Dirichlet Maps," presented at SIAM Conference on Computational Science and Engineering, Atlanta, GA, February 27 – March 3.

L6 F. Rizzi, K. Morris, P. Mycek, K. Sargsyan, O.P. Le Maître, O.M. Knio, A. Contreras, C. Safta, B.J. Debusschere (2016) "A Soft and Hard Faults Resilient Solver for 2D Uncertain Elliptic PDEs via Fault-tolerant MPI Server-client-based Implementation," presented at SIAM Conference on Uncertainty Quantification, Lausanne, Switzerland, April 5-8.

L7 P. Mycek, A. Contreras, O.P. Le Maître, K. Sargsyan, F. Rizzi, K. Morris, C. Safta, B.J. Debusschere, O.M. Knio (2016) "A Hybrid Approach to Tackle Resiliency in Extreme Scale Computations Using a Domain Decomposition Solver for Uncertain Elliptic PDEs," presented at SIAM Conference on Uncertainty Quantification, Lausanne, Switzerland, April 5-8.

L8 P. Mycek, A. Contreras, O.P. Le Maître, K. Sargsyan, F. Rizzi, K. Morris, C. Safta, B.J. Debusschere, O.M. Knio (2016) "A Resilient Domain Decomposition Approach for Extreme Scale UQ Computation," presented at 17th SIAM Conference on Parallel Processing for Scientific Computing, Paris, France, April 12-15.

L9 K. Morris, F. Rizzi, K. Sargsyan, K. Dahlgren, P. Mycek, C. Safta, O.P. Le Maître, O.M. Knio, B.J. Debusschere (2016) "Quantifying Performance of a Resilient Elliptic PDE Solver on Uncertain Architectures Using SST/macro," presented at 17th SIAM Conference on Parallel Processing for Scientific Computing, Paris, France, April 12-15.

L10 F. Rizzi, K. Morris, P. Mycek, O. Le Maître, A. Contreras, K. Sargsyan, C. Safta, O.M. Knio, B.J. Debusschere (2016) "A soft and hard faults resilient solver for 2D elliptic PDEs via server-client-based implementation," presented at 17th SIAM Conference on Parallel Processing for Scientific Computing, Paris, France, April 12-15.

L11 F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. Le Maître, O. Knio, B. Debusschere (2016) "Exploring the Interplay of Resilience and Energy Consumption for a Task-Based Partial Differential Equations Preconditioner," presented at PPoPP16, Barcelona, Spain, Mar 12-16.

L12 F. Rizzi, K. Morris, K. Sargsyan, K. Dahlgren, P. Mycek, C. Safta, O. Le Maître, O. Knio, B. Debusschere (2016)"Scalability of Partial Differential Equations Preconditioner Resilient to Soft & Hard Faults," presented at ISC High Performance 2016, Frankfurt, Germany, June 19-23.

L13 F. Rizzi, K. Sargsyan, K. Morris, C. Safta, P. Mycek, O.M. Knio, O.P. Le Maître, H.N. Najm, B.J. Debusschere (2015) "Spatial Decomposition for Resilient Extreme-Scale Scientific Simulations," presented at SIAM Conference on Computational Science and Engineering, Salt Lake City, UT, March 14–18.

L14 F. Rizzi. K. Morris, K. Sargsyan, C. Safta, P. Mycek, O. Le Maître, O.M. Knio, B.J. Debusschere (2015) "Partial Differential Equations Preconditioner Resilient to Soft and Hard Faults," presented at 1st International Workshop on Fault Tolerant Systems, Chicago, IL, September 8.

L15 P. Mycek, O. P. Le Maître, F. Rizzi, K. Sargsyan, K. Morris, B.J. Debusschere, O.M. Knio (2015) "Parametric Uncertainty Propagation in Resilient Domain Decomposition Methods," presented at SIAM Conference on Computational Science and Engineering, Salt Lake City, UT, March 14–18.

L16 F. Rizzi, K. Sargsyan, K. Morris, O. Knio, P. Mycek, O. Le Maître, C. Safta, H. Najm, B. Debusschere (2014) "Towards a Probabilistic Approach to Extreme-Scale Simulations under Uncertainty and System Faults," presented at SIAM Workshop on Exascale Applied Mathematics Challenges and Opportunities (EX14) Chicago, IL, July 6.

L17 B.J. Debusschere, K. Sargsyan, F. Rizzi, C. Safta, K. Morris, O.M. Knio, H.N. Najm (2014) "Probabilistic Approaches for Fault-Tolerance and Scalability in Extreme-Scale Computing," presented at 16th SIAM Conference on Parallel Processing for Scientific Computing, Portland, OR, February 18–21.

L18 B.J. Debusschere, K. Sargsyan, F. Rizzi, C. Safta, K. Morris, O.M. Knio, H.N. Najm (2014) "Probabilistic Approaches for Fault-Tolerance and Scalability in Extreme-Scale Computing," presented at SIAM UQ 14, Savannah, GA, March 31–April 3.