The Journal of Open Source Software

ASGarD: Adaptive Sparse Grid Discretization

Steven E. Hahn [1], **Miroslav K Stoyanov** [1], **Stefan Schnake** [1], **Eirik Endeve** [1], **David L. Green** [1], **Mark Cianciosa** [1], **Ed D'Azevedo** [1], **Wael Elwasif** [1], **Coleman J. Kendrick** [1], **Hao Lau**[1], **M. Graham Lopez** [1], **Adam McDaniel**[1,4], **B.Tyler McDaniel**[1,2], **Lin Mu** [1,3], **Timothy Younkin** [1], **Hugo Brunie**[5,6,7], **Nestor Demeure**[5,6], **and Cory D Hauck** [1]

1 Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA **2** University of Tennessee Knoxville, Knoxville, Tennessee, USA **3** University of Georgia, Athens, Georgia, USA **4** South Doyle High School, Knoxville, Tennessee, USA **5** National Energy Research Scientific Computing Center, Berkeley, California, USA **6** Lawrence Berkley Laboratory, Berkeley, California, USA **7** National Institute for Research in Digital Science and Technology, France

DOI: 10.21105/joss.06766

Software

- Review
- Repository
- Archive

Editor: Jed Brown

Reviewers:

- @joglekara
- @gnorman7

Submitted: 21 March 2024
Published: 22 August 2024

Summary

Many areas of science exhibit physical processes that are described by high dimensional partial differential equations (PDEs), e.g., the 4D (Dorf et al., 2013), 5D (Candy et al., 2009) and 6D models (Juno et al., 2018) describing magnetized fusion plasmas, models describing quantum chemistry, or derivatives pricing (Bandrauk et al., 2007). Such problems are affected by the so-called "curse of dimensionality" where the number of degrees of freedom (or unknowns) required to be solved for scales as N^D where N is the number of grid points in any given dimension D. A simple, albeit naive, 6D example is demonstrated in the left panel of Figure 1. With $N = 1000$ grid points in each dimension, the memory required just to store the solution vector, not to mention forming the matrix required to advance such a system in time, would exceed an exabyte - and also the available memory on the largest of supercomputers available today. The right panel of Figure 1 demonstrates potential savings for a range of problem dimensionalities and grid resolution. While there are methods to simulate such high-dimensional systems, they are mostly based on Monte-Carlo methods (E et al., 2021), which rely on a statistical sampling such that the resulting solutions include noise. Since the noise in such methods can only be reduced at a rate proportional to $\sqrt{N_p}$ where N_p is the number of Monte-Carlo samples, there is a need for continuum, or grid/mesh-based methods for high-dimensional problems, which both do not suffer from noise and bypass the curse of dimensionality. We present a simulation framework that provides such a method using adaptive sparse grids (Pflüger et al., 2010).

The Adaptive Sparse Grid Discretization (ASGarD) code is a framework specifically targeted at solving high-dimensional PDEs using a combination of a Discontinuous-Galerkin Finite Element solver implemented atop an adaptive sparse grid basis. The adaptivity aspect allows for the sparsity of the basis to be adapted to the properties of the problem of interest, which facilitates retaining the advantages of sparse grids in cases where the standard sparse grid selection rule is not the best match. A prototype of the non-adaptive sparse-grid implementation was used to produce the results of D'Azevedo et al. (2020) for 3D time-domain Maxwell's equations. ASGarD's functionality was recently extended to solve the Vlasov–Poisson–Lenard–Bernstein Model at lower computational cost (Schnake et al., 2024). The implementation utilizes both CPU and GPU resources, as well as being single- and multi-node capable. Performance portability is achieved by casting the computational kernels as linear algebra operations and relying on vendor-provided BLAS libraries. Several test problems are provided, including advection up to 6D with either explicit or implicit timestepping.

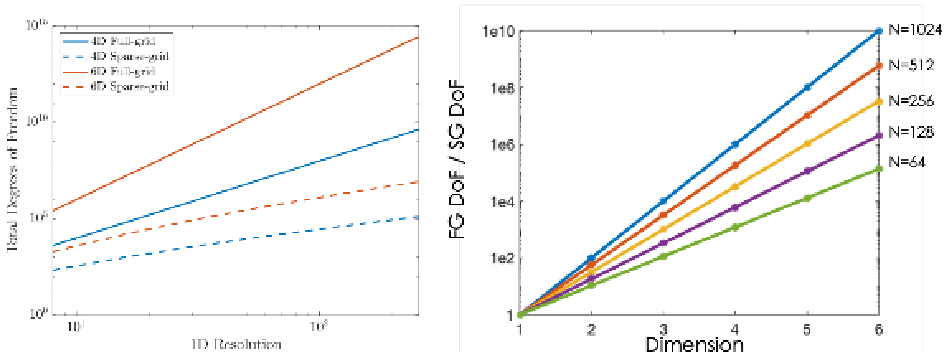

Figure 1: (left) Illustration of the curse of dimensionality in the context of solving a 4 or 6 dimensional PDE (e.g., those at the heart of magnetically confined fusion plasma physics) on modern supercomputers, and how the memory required to store the solution vector for both naive and Sparse Grid based discretizations as the resolution of the simulation domain is varied.; (right) Potential memory savings of a Sparse Grid based solver represented as the ratio of the naive tensor product full-grid (FG) degrees of freedom (DoF) to the sparse-grid (SG) DoF.

Statement of Need

The goal of ASGarD is to facilitate and promote the use of adaptive sparse-grid methods by domain scientists for the approximation of kinetic models. ASGarD provides a robust yet flexible adaptive sparse-grid library for solving PDEs where the "curse-of-dimensionality" and computational complexity previously restricted domain scientists to Monte-Carlo sampling simulation.

State of the Field

While GitHub Topics reports 65 public repositories for the discontinuous-Galerkin method and 13 for sparse-grids, only two combine these two techniques. GalerkinSparseGrids.jl is written in Julia and missing adaptivity, distributed- and shared-memory parallelism or GPU accelerator support (Atanasov & Schnetter, 2017). AdaM-DG is written in C++ and lacks distributed-memory parallelism or GPU accelerator support (Huang et al., 2024).

Acknowledgements

Notice: This manuscript has been authored by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy. The publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a non-exclusive, paid up, irrevocable, world-wide license to publish or reproduce the published form of the manuscript, or allow others to do so, for U.S. Government purposes. The DOE will provide public access to these results in accordance with the DOE Public Access Plan (http://energy.gov/downloads/doe-public-access-plan).

This material is based upon work partially supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, as part of their Applied Mathematics Research Program; the U.S. Department of Energy, Office of Science, Office of Fusion Energy Science as part of their Fusion Research Energy Program; and the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC for the U.S. Department of Energy under Contract No. De-AC05-00OR22725. This research used resources of the Oak Ridge Leadership Computing

Facility (OLCF) at the Oak Ridge National Laboratory, and the National Energy Research Scientific Computing Center (NERSC), which are supported by the Office of Science of the U.S. Department of Energy under Contract Numbers DE-AC05-00OR22725 and DE-AC02-05CH11231 respectively.

References

Atanasov, A. B., & Schnetter, E. (2017). Sparse grid discretizations based on a discontinuous Galerkin method. *arXiv*. https://doi.org/10.48550/arXiv.1710.09356

Bandrauk, A. D., Delfour, M. C., & Le Bris, C. (2007). *High-dimensional partial differential equations in science and engineering* (Vol. 41). American Mathematical Soc. https://doi.org/10.1090/crmp/041

Candy, J., Holland, C., Waltz, R. E., Fahey, M. R., & Belli, E. (2009). Tokamak profile prediction using direct gyrokinetic and neoclassical simulation. *Physics of Plasmas*, *16*(6), 060704. https://doi.org/10.1063/1.3167820

D'Azevedo, E., Green, D. L., & Mu, L. (2020). Discontinuous Galerkin sparse grids methods for time domain Maxwell's equations. *Computer Physics Communications*, *256*, 107412. https://doi.org/10.1016/j.cpc.2020.107412

Dorf, M. A., Cohen, R. H., Dorr, M., Rognlien, T., Hittinger, J., Compton, J., Colella, P., Martin, D., & McCorquodale, P. (2013). Simulation of neoclassical transport with the continuum gyrokinetic code COGENT. *Physics of Plasmas*, *20*(1), 012513. https://doi.org/10.1063/1.4776712

E, W., Han, J., & Jentzen, A. (2021). Algorithms for solving high dimensional PDEs: From nonlinear Monte Carlo to machine learning. *Nonlinearity*, *35*(1), 278. https://doi.org/10.1088/1361-6544/ac337f

Huang, J., Guo, W., & Cheng, Y. (2024). Adaptive sparse grid discontinuous Galerkin method: Review and software implementation. *Communications on Applied Mathematics and Computation*, *6*, 501–532. https://doi.org/10.1007/s42967-023-00268-8

Juno, J., Hakim, A., TenBarge, J., Shi, E., & Dorland, W. (2018). Discontinuous Galerkin algorithms for fully kinetic plasmas. *Journal of Computational Physics*, *353*, 110–147. https://doi.org/10.1016/j.jcp.2017.10.009

Pflüger, D., Peherstorfer, B., & Bungartz, H.-J. (2010). Spatially adaptive sparse grids for high-dimensional data-driven problems. *Journal of Complexity*, *26*(5), 508–522. https://doi.org/10.1016/j.jco.2010.04.001

Schnake, S., Kendrick, C., Endeve, E., Stoyanov, M., Hahn, S., Hauck, C. D., Green, D. L., Snyder, P., & Canik, J. (2024). Sparse-grid discontinuous Galerkin methods for the Vlasov–Poisson–Lenard–Bernstein model. *Journal of Computational Physics*, *510*, 113053. https://doi.org/10.1016/j.jcp.2024.113053