

Spiner: Performance Portable Routines for Generic, Tabulated, Multi-Dimensional Data

Jonah M. Miller^{*1,2}, Daniel Holladay^{2,3}, Chad D. Meyer⁴, Joshua C. Dolence^{1,2}, Sriram Swaminarayan³, Christopher M. Mauney^{2,5}, and Karen Tsai³

¹ CCS-2, Computational Physics and Methods, Los Alamos National Laboratory, Los Alamos, NM ² Center for Theoretical Astrophysics, Los Alamos National Laboratory, Los Alamos, NM ³ CCS-7, Applied Computer Science, Los Alamos National Laboratory, Los Alamos, NM ⁴ XCP-4, Continuum Models and Numerical Methods, Los Alamos National Laboratory, Los Alamos, NM ⁵ HPC-ENV, HPC Environments, Los Alamos National Laboratory, Los Alamos, NM

DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

Software

- [Review](#)
- [Repository](#)
- [Archive](#)

Editor: [✉](#)

Submitted: 17 March 2022

Published: unpublished

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](#)).

Summary

We present Spiner, a new, performance-portable library for working with tabulated data. Spiner provides efficient routines for multi-dimensional interpolation and indexing on CPUs and GPUs, including interwoven interpolation and indexing access patterns, as needed for radiation transport. Importantly, Spiner defines a data format, based on HDF5, that couples the tabulated data to the information required to interpolate it, which Spiner can read and move to GPU.

Statement of Need

As Moore's law comes to an end, more and more performance comes from specialized hardware, such as GPUs. A key tool in the toolbox for many scientific codes is tabulated data. Fluid and continuum dynamics codes often encapsulate the equation of state as data tabulated in density and temperature, for example as published in the Sesame database ([Lyon & Johnson, 1992](#)) or the stellar collapse database ([O'Connor & Ott, 2010b](#)), first presented in ([O'Connor & Ott, 2010a](#)). Radiation transport, such as that performed by ([Skinner et al., 2019](#)) and ([Miller et al., 2019](#)) uses emissivity and absorption opacity on tables such as those computed in ([Sullivan et al., 2016](#)). Spiner is now used in the open-source and on-going Singularity-EOS ([The Singularity Team, 2022a](#)), Singularity-Opac ([The Singularity Team, 2022b](#)), and Phoebus ([The Phoebus Team, 2022](#)) projects, which have separate code papers in-prep.

State of the Field

Interpolation is a common problem, implemented countless times across software projects, and a core part of any introductory text on scientific computing ([Press et al., 2007](#)), however, a performance-portable implementation not tuned to a specific use-case or embedded in a larger project is (to our knowledge) not available in the literature. A common problem in performance-portable computing is the management of performance-portable data structures. Libraries, such as Kokkos ([Trott et al., 2022](#)), often provide this functionality.

Here we present Spiner, a performance-portable library for working with tabulated data, thus meeting the needs of simulation codes on emerging hardware. Spiner provides data structures

^{*}jonahm@lanl.gov

for working with tabulated data on both CPU and GPU, routines for interpolating on and indexing into tabulated data, and a file format that couples data to the information required to interpolate it. Spiner therefore fills a gap in available open software, providing a needed service for GPU simulation codes.

Design Principles and Salient Features

We built Spiner with several design goals in mind. First and foremost, interpolation must be fast, sufficiently fast that interpolation operations are not the rate-limiting operation in a larger calculation. Second, Spiner must be lightweight. It should contain exactly enough features to be useful for relevant science applications. Similarly, Spiner must be sufficiently low-level and flexible that it can support all performance portability strategies and access patterns required of it. That said, not all needs will be known at conception, and needs change over time. Thus Spiner must be extendable. Finally, Spiner should be well-documented with a modern, easy-to-use build system. We believe we have achieved these goals.

To ensure Spiner is lightweight and performant, it is header-only. To ensure performance portability, we rely on the Kokkos (Trott et al., 2022) library to provide performance portable data structures and parallel dispatch. However, we recognize that another performance portability paradigm may be desired. Hence, we developed a separate library, Ports-of-Call, which we open-sourced at (The Ports-of-Call Team, 2022). Ports-of-Call is a very thin abstraction around low-level device calls. It provides preprocessor macros to enable or disable Kokkos, an arbitrary-dimensional array data structure, and hooks to add the same functionality for other backends such as pure CPU, OpenMP (Chandra et al., 2001), or Cuda (NVIDIA et al., 2020). Ports-of-Call is only a few hundred lines long. Both Spiner and Ports-of-Call are well documented, with Sphinx documentation provided automatically by github pages and github actions. They both also have modern build systems, with Cmake and Spack support. Unit tests are provided by Catch2 (The Catch2 Collaboration, 2013).

The fundamental data structures are the DataBox and RegularGrid1D. The former relies heavily on the PortableMDArray data structure in Ports-of-Call for data storage, which provides an arbitrary-dimensional accessor to a contiguous block of data, as well as support for slicing, shallow copying, and resizing data. The latter contains information required to interpolate. The former contains both the data to interpolate, as well as multiple RegularGrid1Ds. Both objects know how to read from and write to an HDF5 (The HDF Group, 2000) file, and the intent is that the RegularGrid1D is a hook that could be extended into a more sophisticated gridding or interpolation procedure. A DataBox can manage its own memory and can automatically allocate on host or device at runtime. Deep copies host-to-host and host-to-device are supported. To encourage good performance, no deep copies are ever implicitly performed—they must be explicitly requested. Consequently, DataBoxes have reference semantics. By deliberate choice, DataBoxes are not reference-counted and have trivial destructors. Instead, we provide an overload of free to free the data. However, DataBoxes can be managed via smart pointers—and we provide machinery to do so. We find this approach minimizes code complexity and carries most of the benefits of an automatically reference-counted data structure.

Performance And Accuracy

Since it is usually sufficient for the intended use-cases, only multilinear interpolation is supported, although as discussed above, hooks are present in the code for more sophisticated approaches. A convergence test is available in the test suite and shows excellent second-order convergence as expected. Performance on both CPUs and GPUs is also excellent. For example, the figure below benchmarks trilinear interpolation from a 64^3 grid on to a cubic grid of varying sizes. We test on a single Intel Xeon (Haswell) core, twenty cores accross two sockets (with a Kokkos OpenMP backend), and one Nvidia V100 GPU (with the Kokkos Cuda backend). We find an

86 8x speedup going from 1 core to two full sockets. This number can be likely improved with
87 tuning of the Kokkos OpenMP backend. We also find that after the V100 GPU saturates, it
88 offers an approximately 300x speedup over the serial calculation.

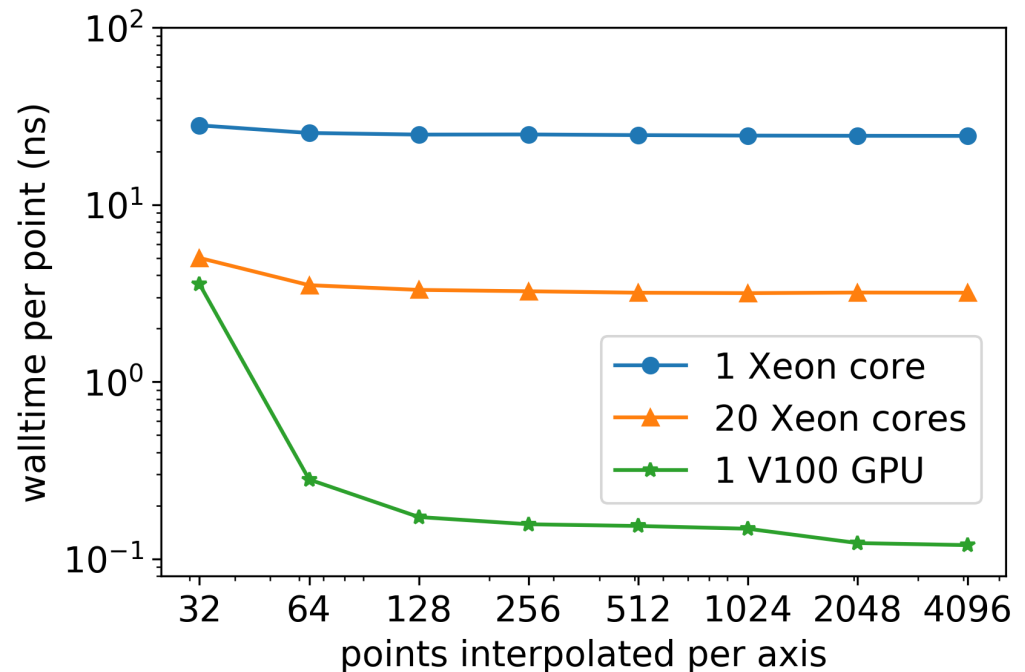


Figure 1: Performance of trilinear interpolation on one Haswell core, twenty Haswell cores, and a V100 GPU. Smaller is better. The rightmost point is over 68 billion interpolation operations.

Acknowledgements

This work was supported by the U.S. Department of Energy through the Los Alamos National Laboratory (LANL). LANL is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001). This research used resources provided by the Darwin testbed at LANL which is funded by the Computational Systems and Software Environments subprogram of LANL's Advanced Simulation and Computing program (NNSA/DOE). This work is approved for unlimited release with report number LA-UR-22-22502.

Chandra, R., Dagum, L., Kohr, D., Menon, R., Maydan, D., & McDonald, J. (2001). *Parallel programming in OpenMP*. Morgan kaufmann.

Lyon, S. P., & Johnson, J. D. (1992). *Sesame: The los alamos national laboratory equation of state database* (LA-UR-92-3407). Los Alamos National Laboratory.

Miller, J. M., Ryan, Ben. R., & Dolence, J. C. (2019). ν bhlight: Radiation GRMHD for Neutrino-driven Accretion Flows. *241*(2), 30. <https://doi.org/10.3847/1538-4365/ab09fc>

NVIDIA, Vingelmann, P., & Fitzek, F. H. P. (2020). *CUDA, release: 10.2.89*. <https://developer.nvidia.com/cuda-toolkit>

O'Connor, E., & Ott, C. D. (2010a). A new open-source code for spherically symmetric stellar collapse to neutron stars and black holes. *Classical and Quantum Gravity*, *27*(11), 114103. <https://doi.org/10.1088/0264-9381/27/11/114103>

- 108 O'Connor, E., & Ott, C. D. (2010b). *Stellar collapse: microphysics*. <https://stellarcollapse.org/equationofstate>
- 109
- 110 Press, W. H., Teukolsky, S. A., Vetterling, W. T., & Flannery, B. P. (2007). *Numerical recipes with source code CD-ROM 3rd edition: The art of scientific computing*. Cambridge University Press. ISBN: 9780521884075
- 111
- 112
- 113 Skinner, M. A., Dolence, J. C., Burrows, A., Radice, D., & Vartanyan, D. (2019). FORNAX: A Flexible Code for Multiphysics Astrophysical Simulations. *241*(1), 7. <https://doi.org/10.3847/1538-4365/ab007f>
- 114
- 115
- 116 Sullivan, C., O'Connor, E., Zegers, R. G. T., Grubb, T., & Austin, S. M. (2016). The Sensitivity of Core-collapse Supernovae to Nuclear Electron Capture. *816*(1), 44. <https://doi.org/10.3847/0004-637X/816/1/44>
- 117
- 118
- 119 The Catch2 Collaboration. (2013). Catch2. In *GitHub repository*. GitHub. <https://github.com/catchorg/Catch2>
- 120
- 121 The HDF Group. (2000). *Hierarchical data format version 5*. <http://www.hdfgroup.org/HDF5>
- 122
- 123 The Phoebus Team. (2022). Phoebus: Phifty one ergs blows up a star. In *GitHub repository*. GitHub. <https://github.com/lanl/phoebus>
- 124
- 125 The Ports-of-Call Team. (2022). Ports-of-call. In *GitHub repository*. GitHub. <https://github.com/lanl/ports-of-call>
- 126
- 127 The Singularity Team. (2022a). Singularity-EOS: Performance portable equations of state. In *GitHub repository*. GitHub. <https://github.com/lanl/singularity-eos>
- 128
- 129 The Singularity Team. (2022b). Singularity-opac: Performance portable opacities. In *GitHub repository*. GitHub. <https://github.com/lanl/singularity-opac>
- 130
- 131 Trott, C. R., Lebrun-Grandié, D., Arndt, D., Ciesko, J., Dang, V., Ellingwood, N., Gayatri, R., Harvey, E., Hollman, D. S., Ibanez, D., Liber, N., Madsen, J., Miles, J., Poliakov, D., Powell, A., Rajamanickam, S., Simberg, M., Sunderland, D., Turcksin, B., & Wilke, J. (2022). Kokkos 3: Programming model extensions for the exascale era. *IEEE Transactions on Parallel and Distributed Systems*, *33*(4), 805–817. <https://doi.org/10.1109/TPDS.2021.3097283>
- 132
- 133
- 134
- 135