

shmem4py: OpenSHMEM for Python

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Summary

shmem4py brings the Partitioned Global Address Space (PGAS) programming model to Python by exposing the functionality of the OpenSHMEM Application Programming Interface (API) specification. The feature set includes one-sided communication, shared memory access, atomic memory operations, and collective operations. The Python implementation of shmem4py emphasizes using NumPy arrays, providing convenient access to the symmetric memory allocations central to OpenSHMEM's programming model. Thanks to Python's versatility and OpenSHMEM implementations' focus on performance, shmem4py offers a seamless experience on a variety of hardware, from laptops to supercomputers, and for a wide range of applications and users. shmem4py API grounds in OpenSHMEM 1.5 specification; however, it also supports legacy 1.4 implementations.

Statement of Need

Python applications can be scaled to multiple processes and compute nodes in various ways. When working on a single node, the multiprocessing or concurrent futures packages from the Python standard library offer solutions for task-based parallelism. As we expand beyond a single node, more advanced frameworks like Dask (Rocklin, 2015), Ray (Moritz et al., 2018) or mpi4py.futures (Rogowski et al., 2023) are commonly used. Typically, these high-level frameworks handle interprocess communication transparently to the user.

More challenging applications often require specialized communication patterns. In those cases, Python applications can leverage communication frameworks originally designed for high-performance computing. One such example is mpi4py (Dalcin & Fang, 2021), which offers MPI bindings for Python. shmem4py adopts a similar approach, providing Python bindings to OpenSHMEM (Chapman et al., 2010) implementations with a Python-centric and high-level API built on top of a low-level CFFI (Rigo & Fijalkowski, 2022) module. This way, shmem4py is accessible to a diverse audience while offering a proven programming model with reliable performance.

shmem4py complements mpi4py in the same way that OpenSHMEM complements MPI. MPI is extremely popular in high-performance computing because of its combination of a rich feature set and generality. OpenSHMEM is based on a different philosophy, which provides a smaller set of features that better match high-performance computing system hardware capabilities. For example, OpenSHMEM one-sided communication and atomic operations are aligned with networking capabilities such as remote direct memory access (RDMA) such that no intervention is required on the remote side (Jose et al., 2014). In contrast, MPI's one-sided communication functionality includes many more features, some of which are known to make implementations based strictly on RDMA more difficult (Hammond et al., 2014; Si et al., 2015). Another aspect of the tradeoff between generality and close-to-hardware features is observed in the



context of specialized processors, such as GPUs. It has been shown that OpenSHMEM-like APIs can be implemented natively on GPUs, e.g., NVSHMEM (Hsu et al., 2020; Potluri et al., 2017). On the other hand, implementing MPI send and receive operations in the same context poses significant challenges. In fact, shmem4py will provide the backbone for future extensions supporting inter-GPU communication.

We envision two distinct groups of users that may be interested in shmem4py. The first, and likely most numerous, group includes Python programmers who lack the expertise or the time to write low-level code in C and have applications well-suited for the PGAS paradigm. The second group comprises high-performance computing professionals familiar with OpenSHMEM who want to prototype or port parts of their applications to Python. Both groups of users can benefit greatly from the ease of development in Python, shmem4py's convenience functions for manipulating NumPy arrays in symmetric memory, and all of OpenSHMEM features. We also expect that current users of mpi4py may want to try shmem4py as a complementary communication model for the same reasons that OpenSHMEM is used alongside MPI.

Supported OpenSHMEM Implementations

The shmem4py package supports, and is tested with, all major implementations of the Open-SHMEM specification:

- Cray OpenSHMEMX
- Open MPI OpenSHMEM
- Open Source Software Solutions (OSSS) OpenSHMEM
- OSHMPI
- Sandia OpenSHMEM

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