OPS-SENGA+: A Performance-Portable Solver for High-Fidelity Reacting Flow Simulations on CPUs and GPUs

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SENGA+ [1] is a well-established high-order finite-difference solver for direct numerical simulation (DNS) of reactive flows. It was originally developed targeting distributed-memory CPU systems. With the growing trend in high-performance computing (HPC) toward accelerator-based systems, particularly GPUs, in leading supercomputing centers, there is a pressing need to adapt legacy solvers for these platforms. In this work, we re-engineer the SENGA+ code to utilize GPUs using the Oxford Parallel library for Structured-mesh solvers (OPS) [2] domain specific language (DSL), enabling performance-portable execution while preserving the solver's original accuracy and algorithmic structure. The new code is extensively validated to assure accuracy and precision. The first validation case is a one-dimensional freely propagating laminar hydrogen-air premixed flames over a range of equivalence ratios. The re-engineered OPS-SENGA+ accurately reproduces the temperature and species mass fraction profiles in excellent agreement with both the original version. To validate the correctness and fidelity in at production-representative scale, a 3D Taylor-Green Vortex (TGV) configuration is used next in both non-reacting and reacting modes. For the non-reacting case, the OPS-ported solver accurately captured the evolution of volume-integrated enstrophy and turbulent kinetic energy, matching both the original code's results and established reference data. The reacting TGV case incorporated a multi-species hydrogen-air mixture with an embedded flame zone. The temporal evolution of maximum temperature and species distributions has an excellent agreement between both versions, confirming the solver's correctness under coupled turbulent-chemistry interactions. These cases establish that the GPU-enabled SENGA+ preserves accuracy and robustness across reacting flow regimes. The significant advantage of the new GPU-enabled code can be seen from the up to 4x speed-up over the baseline of the original MPI-only version. Additionally, we see excellent scaling both strong and weak on up to 4096 GPUs. The new code's capabilities point to a step change in time-to-solution of SENGA+ simulations, enabling production-level combustion problems to be solved at high-fidelity within tractable timeframes that were previously prohibitively expensive.

References

[1] R. S. Cant. 2012. SENGA2 User Guide. Technical Report CUED-THERMO-2012/04 (2nd ed.). Cambridge University Engineering Department, Cambridge, UK.
[2] I. Z. Reguly, G. R. Mudalige and M. B. Giles, Loop Tiling in Large-Scale Stencil Codes at Run-Time with OPS, in IEEE Transactions on Parallel and Distributed Systems, vol. 29, no. 4, pp. 873-886, 1 April 2018.