The Journal of Open Source Software

NebulaSEM: A high-order discontinuous Galerkin spectral element code for atmospheric modeling

Daniel S. Abdi[1¶]

1 Cooperative Institute for Research in Environmental Sciences ¶ Corresponding author

DOI: 10.xxxxxx/draft

Software

- Review
- Repository
- Archive

Editor:

Submitted: 21 December 2023
Published: unpublished

Summary

NebulaSEM is an advanced computational fluid dynamics (CFD) model employing the high-order discontinuous Galerkin spectral elementi (dGSEM) method. Originally designed for generic CFD applications with polyhedral elements on unstructured grids, NebulaSEM has recently evolved into an atmospheric simulation code. This paper presents the key features, capabilities, and applications of NebulaSEM, highlighting its high-order discretization, oct-tree cell-based adaptive mesh refinement (AMR), support for new solver development, turbulence models, and parallelization strategies. The software addresses the need for high-fidelity simulations in diverse areas, offering an efficient and scalable solution with a focus on atmospheric modeling.

NebulaSEM Features

High-order dGSEM discretization

NebulaSEM supports arbitrarily high-order discontinuous Galerkin spectral element discretization of PDEs besides finite-volume discretization, which is a subset of dGSEM with the lowest polynomial order of zero. The spectral element discretization is significantly more efficient than standard discontinuous Galerkin on unstructured grid because the former exploits the tensor-product nature of computations to reduce computations from O(N^3) to O(3N). The dGSEM possesses several desirable characteristics (D. S. Abdi et al., 2017) such as: high-order accuracy, geometrical flexibility compared to global spectral methods, high scalability due to the high arithmetic intensity per element, suitability for GPU acceleration, and support for both h- and p- refinement.

Oct-tree cell-based AMR

Modeling of the atmosphere is challenging in that a range of spatial and temporal scales are involved (Wallace & Hobbs, 2006). Adaptive Mesh Refinement (AMR) provides the tool to address multi-scale phenomenon efficiently by focusing resources where they are needed. NebulaSEM implements oct-tree cell-based AMR using the forest-of-octrees approach pioneered in (Burstedde et al., 2011). The `AmrIteration` class provides a high-level interface to enable AMR for any solver written using the library. A single loop enclosing the timestep iterations and declaration of fields involved in the PDE is enough to provide AMR capability for any solver. The details of regridding the domain, memory management, resizing and transferring fields in a conservative manner etc are all taken care of behind the scenes by the library.

Support for new solver development

NebulaSEM offers a range of operators for spatial and temporal discretization, streamlining the development of solvers for Partial Differential Equations (PDEs). The provided code snippet includes an example solver for the advection-diffusion equation.

```
void transport() {
    for (AmrIteration ait; !ait.end(); ait.next()) {     /*AMR iteration object (ait) an
         VectorCellField U("U", READWRITE);              /*Velocity field defined over
         ScalarCellField T("T", READWRITE);              /*Scalar field*/
         ScalarFacetField F = flx(U);                    /*Compute flux field*/
         ScalarCellField mu = 1;                         /*Diffusion parameter*/
         for (Iteration it(ait.get_step()); !it.end(); it.next()) { /*Time loop with sup
             ScalarCellMatrix M;                         /*Matrix for the PDE discretiz
             M = div(T,U,F,&mu) - lap(T,mu);             /*Divergence & Laplacian terms
             addTemporal<1>(M);                          /*Add temporal derivative*/
             Solve(M);                                   /*Solve the matrix */
         }
    }
}
```

Spatial operators within dGSEM encompass divergence, gradient, laplacian, and more. Temporal discretization is accomplished through explicit and implicit schemes, including first-order Euler explicit and implicit schemes, linear multi-step methods such as Adams-Moulton and Adams-Bashforth, the Runge-Kutta method up to 4th order, and fully-implicit Backward Differencing (BDF) methods.

Turbulence models

The software includes turbulence models for high-Reynolds CFD simulations including a suite of Reynolds Averaged Navier Stokes (RANS) (Tennekes & Lumley, 1972) and Large Eddy Simulation (LES) models (Nakanishi & Niino, 1963). The list includes a mixing-length model, k-epsilon, k-omega, RNG k-epsilon, RNG k-omega and the Smagornisky-Lilly LES model. Theese turbulence models has been utilized to evaluate the aerodynamic roughness of the built environment and complex terrain in (D. Abdi & Bitsuamlak, 2014).

Parallelization with MPI+OpenMP/OpenACC

NebulaSEM achieves scalability on supercomputers through a combination of coarse- and fine-grained parallelism. The Message Passing Interface (MPI) is employed for distributed computing, while directive-based threading libraries such as OpenMP for CPUs and OpenACC for GPUs optimize fine-grained parallelism, minimizing communication overhead. Details of parallelization of the linear system of equations solvers, such as the preconditioned gradient solver, can be found in (D. Abdi & Bitsuamlak, 2015). In addition, NebulaSEM implements a unique approach of asynchronous parallelization that is not commonly found in CFD applications.

Efficient GPU implementation of dGSEM is achieved through offloading of all field computations to the GPU (D. S. Abdi et al., 2017), using a memory pool to recycle previously allocated memory by fields that went out of scope, utilization of managed memory to simplify the data transfer logic between CPU and GPU etc.

Showcases

We showcase the capabilities of NebulaSEM through two example applications:

a) Generic CFD Application: We employ the Pressure-Implicit Splitting of Operators (PISO) solver for incompressible fluid flow to solve the Pitz-Daily problem (Pitz & Daily, 1983), utilizing the Smagornisky-Lilly large eddy simulation. The instantaneous velocity profiles are depicted in Figure 1.

b) Atmospheric Simulation: NebulaSEM can serve as a non-hydrostatic dynamical core for atmospheric simulation. To evaluate the dynamical core, we solve the rising thermal bubble problem (Robert, 1993) using the non-hydrostatic Euler equations solver. The test involves adaptive mesh refinement and discontinuous Galerkin spectral element discretization with polynomial order of 4. The result is depicted in Figure 2

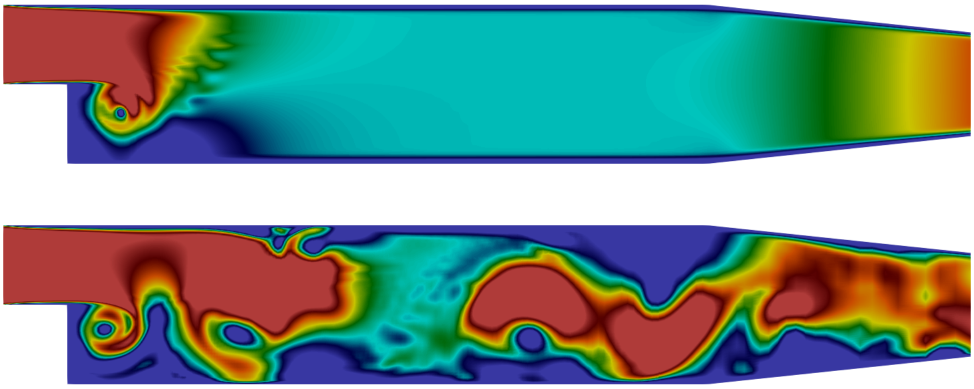

Figure 1: Simulation results for the Pitz-Daily problem (Pitz & Daily, 1983) that aims to evaluate the effect of combustion on mixing layer growth. A snapshot of large eddy simulation (LES) results using finite-volume method of NebulaSEM is presented.

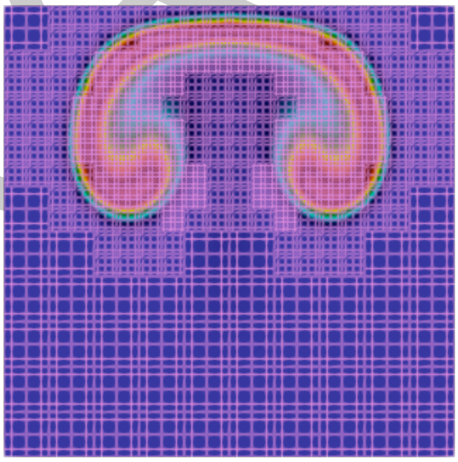

Figure 2: Simulation results for the Robert Rising Thermal Bubble (RRTB) problem (Robert, 1993) using oct-tree cell-based AMR with two levels of refinement. The discontinuous Galerkin spectral element method is used with polynomial order of 4.

Statement of need

Over the years, NebulaSEM has undergone a transformation from being a purely Computational Fluid Dynamics (CFD) application to primarily serve as an atmospheric simulation (AtmoSim) code. Consequently, it addresses specific needs inherent to both types of applications, as outlined below.

Many CFD codes prioritize robustness over other considerations. As a result, they often utilize first or at best second-order accurate finite volume methods on unstructured grids. In contrast, NebulaSEM offers high-order discretization characterized by high accuracy and minimal dissipation. This feature proves invaluable for tasks such as accurately capturing shocks and discontinuities, conducting highly accurate large eddy simulations, simulating turbulent flows with precision, and facilitating high-fidelity aeroacoustic simulations.

While high-order methods are more commonly associated with atmospheric modeling, such endeavors often rely on finite-difference discretization, which is less geometrically flexible, or global spectral methods on latitude-longitude grids, which lack scalability. NebulaSEM provides geometrical flexibility due to its CFD roots, allowing atmospheric simulaitons on any type of grid. The element-based design, as opposed to global spectral-methods, ensures high-scalability for large scale simulations. The high-order dGSEM discretization it employs delivers the accuracy necessary for achieving high-fidelity atmospheric simulations. In addition, NebulaSEM incorporates dynamic adaptive mesh refinement capabilities, a feature not commonly found in traditional atmospheric modeling approaches.

Acknowledgements

I would like to thank my postdoc supervisor Francis X. Giraldo who introduced me to the high-order discontinuous Galerkin method.

References

Abdi, D. S., Wilcox, L. C., Warburton, T. C., & Giraldo, F. X. (2017). A GPU-accelerated continuous and discontinuous galerkin non-hydrostatic atmospheric model. *The International Journal of High Performance Computing Applications*, *22*, 1094342017694427. https://doi.org/10.1177/1094342017694427

Abdi, D., & Bitsuamlak, G. (2014). Wind flow simulations on idealized and real complex terrain using various turbulence models. *Advances in Engineering Software*, *75*, 30–41. https://doi.org/10.1016/j.advengsoft.2014.05.002

Abdi, D., & Bitsuamlak, G. (2015). Asynchronous parallelization of a CFD solver. *Journal of Computational Engineering*. https://doi.org/10.1155/2015/295393

Burstedde, C., Wilcox, L. C., & Ghattas, O. (2011). `p4est`: Scalable algorithms for parallel adaptive mesh refinement on forests of octrees. *SIAM Journal on Scientific Computing*, *33*(3), 1103–1133. https://doi.org/10.1137/100791634

Nakanishi, M., & Niino, H. (1963). General circulation experiments with the primitive equations. *Mon. Weather Rev.*, *91*, 99–164. https://doi.org/10.1175/1520-0493(1963)091%3C0099:GCEWTP%3E2.3.CO;2

Pitz, R. W., & Daily, J. W. (1983). Combustion in a turbulent mixing layer formed at a rearward-facing step. *AIAA Journal*, *21*(11), 1565–1570. https://doi.org/10.2514/3.8290

Robert, A. (1993). Bubble convection experiments with a semi-implicit formulation of the euler equations. *Journal of Atmospheric Sciences*, *50*(13), 1865–1873. https://doi.org/https://doi.org/10.1175/1520-0469(1993)050%3C1865:BCEWAS%3E2.0.CO;2

Tennekes, H., & Lumley, J. L. (1972). *A First Course in Turbulence*. The MIT Press. https://doi.org/10.7551/mitpress/3014.001.0001

Wallace, J. M., & Hobbs, P. V. (2006). *Atmospheric science: An introductory survey*. Elsevier Academic Press. ISBN: 9780127329512