

### **Summary Version**

Results and benchmark tarball are for the cts2 version from the <u>CEED/Laghos</u> repository.

# Purpose of Benchmark

**Laghos** (LAGrangian High-Order Solver) is a miniapp that solves the time-dependent Euler equations of compressible gas dynamics in a moving Lagrangian frame using unstructured high-order finite element spatial discretization and explicit high-order time-stepping.

Laghos is based on the discretization method described in the following article:

V. Dobrev, Tz. Kolev and R. Rieben <u>High-order curvilinear finite element methods for Lagrangian hydrodynamics</u> *SIAM Journal on Scientific Computing*, (34) 2012, pp. B606-B641

Laghos captures the basic structure of many other compressible shock hydrocodes, including the <u>BLAST code</u> at <u>Lawrence Livermore National Laboratory</u>. The miniapp is built on top of a general discretization library, <u>MFEM</u>, thus separating the pointwise physics from finite element and meshing concerns.

Laghos is a <u>LLNL ASC co-design mini-app</u> that was developed as part of the <u>CEED software suite</u>, a collection of software benchmarks, miniapps, libraries and APIs for efficient exascale discretizations based on high-order finite element and spectral element methods. See <u>http://github.com/ceed</u> for more information and source code availability.

The CEED research is supported by the <u>Exascale Computing Project</u> (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a <u>capable exascale</u> <u>ecosystem</u>, including software, applications, hardware, advanced system engineering and early testbed platforms, in support of the nation's exascale computing imperative.

# Characteristics of Benchmark

In each time step, the problem is ultimately formulated as solving a big system of ordinary differential equations (ODE) for the unknown (high-order) velocity, internal energy and mesh nodes (position). The left-hand side of this ODE is controlled by *mass matrices* (one for velocity and one for energy), while the right-hand side is constructed from a *force matrix*.



Laghos supports two options for deriving and solving the ODE system, namely the *full assembly* and the *partial assembly* methods. **Partial assembly is the main algorithm of interest for this benchmark.** 

Other computational motives in Laghos include the following:

- Support for unstructured meshes, in 2D and 3D, with quadrilateral and hexahedral elements (triangular and tetrahedral elements can also be used, but with the less efficient full assembly option). Serial and parallel mesh refinement options can be set via a command-line flag.
- Explicit time-stepping loop with a variety of time integrator options. Laghos supports Runge-Kutta ODE solvers of orders 1, 2, 3, 4 and 6, as well as a specialized Runge-Kutta method of order 2 that ensures exact energy conservation on fully discrete level (RK2Avg).
- Continuous and discontinuous high-order finite element discretization spaces of runtimespecified order.
- Moving (high-order) meshes.
- Separation between the assembly and the quadrature point-based computations.
- Point-wise definition of mesh size, time-step estimate and artificial viscosity coefficient.
- Constant-in-time velocity mass operator that is inverted iteratively on each time step. This is an example of an operator that is prepared once (fully or partially assembled) but is applied many times. The application cost is dominant for this operator.
- Time-dependent force matrix that is prepared every time step (fully or partially assembled) and is applied just twice per "assembly". Both the preparation and the application costs are important for this operator.
- Domain-decomposed MPI parallelism.
- Optional in-situ visualization with <u>GLVis</u> and data output for visualization / data analysis with <u>VisIt</u>.

### Mechanics of Building the Benchmark

For this run, Laghos has the following external dependencies:

- *hypre*, used for parallel linear algebra, we recommend version 2.10.0b <u>https://computation.llnl.gov/casc/hypre/software.html</u>
- **MFEM**, used for (high-order) finite element discretization, GitHub tag laghos-cts2 <u>https://github.com/mfem/mfem</u>



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- **METIS**, used for parallel domain decomposition, we recommend <u>version 4.0.3</u> <u>http://glaros.dtc.umn.edu/gkhome/metis/metis/download</u>
- **RAJA**, used for handling the kernel's for-loop bodies <u>https://github.com/LLNL/RAJA</u>

Build *hypre* from <u>https://computation.llnl.gov/projects/hypre-scalable-linear-solvers-multigrid-</u>methods/download/hypre-2.10.0b.tar.gz:

```
~> tar xzvf hypre-2.10.0b.tar.gz
~> cd hypre-2.10.0b/src/
~/hypre-2.10.0b/src> ./configure --disable-fortran
~/hypre-2.10.0b/src> make -j
~/hypre-2.10.0b/src> cd ../..
```

Build metis from <a href="http://glaros.dtc.umn.edu/gkhome/fetch/sw/metis/OLD/metis-4.0.3.tar.gz">http://glaros.dtc.umn.edu/gkhome/fetch/sw/metis/OLD/metis-4.0.3.tar.gz</a>

```
~> tar xzvf metis-4.0.3.tar.gz
~> cd metis-4.0.3
~/metis-4.0.3> make
~/metis-4.0.3> cd ..
~/metis-4.0.3> mv metis-4.0.3 metis-4.0
```

Build RAJA from https://github.com/LLNL/RAJA/releases/download/v0.7.0/RAJA-0.7.0.tar.gz:

Build **MFEM** from: <u>https://github.com/mfem/mfem/archive/laghos-cts2.tar.gz</u>:

```
~> tar xzvf mfem-laghos-cts2.tar.gz
~> cd mfem-laghos-cts2/
~/mfem-laghos-cts2> make parallel MFEM_USE_RAJA=YES -j
~/mfem-laghos-cts2> cd ..
~/mfem-laghos-cts2> mv mfem-laghos-cts2 mfem
```

Build Laghos from: <a href="https://github.com/CEED/Laghos/archive/cts2.tar.gz">https://github.com/CEED/Laghos/archive/cts2.tar.gz</a>

- ~> tar xzvf Laghos-cts2.tar.gz
- ~> cd Laghos-cts2/
- ~> make -j

This can be followed by make test to check the build respectively. See make help for additional options.



#### Mechanics of Running the 2D Benchmark Sedov Blast

The main problem of interest for Laghos is the Sedov blast wave  $(-p \ 1)$  with partial assembly option (-pa) and the RAJA backend, accessible through the okina options  $(-o \ -q \ -ra)$ .

A sample runs in 2D is:

mpirun -n 4 laghos -p 1 -m data/square01 quad.mesh -rs 2 -o -q -ra

To partition an initial 2D mesh in a way that results in a perfectly balanced partitioning, with each MPI task having the same number of zones, one needs to specify the correct partitioning ( $-c \quad X \quad Y'$ ) and initial mesh (-m) options. The cartesian partitioning option specifies the relative ratio between the number of MPI tasks in each of the (X, Y) directions.

Furthermore, the number of serial refinements (option -rs) should be sufficiently high to produce at least one zone per MPI task, before the parallel refinements (option -rp) are performed. The data/square\_10x9\_quad mesh has initially 90 zones and with 36 MPI tasks, one should use at least one serial refinement and the (4,9) cartesian partitioning:

```
mpirun -n 36 laghos -p 1 -m data/square_10x9_quad.mesh -rs 1 -rp 0 -o
-q -ra -c '4 9'
```

Other options allow to run on different ranks with a perfectly balanced partitioning: **64** (-rs 3 -rp 0 -c '8 8'), **90** (-rs 1 -rp 2 -c '10 9'), **96** (-rs 2 -rp 1 -c '8 12'), **120** (-rs 1 -rp 2 -c '20 6') and **128** (-rs 3 -rp 0 -c '16 8').

### Verification of Results

To make sure the results are correct, we tabulate reference final iterations (step), time steps (dt) and energies (|e|) for the following runs:

```
mpirun -np 4 laghos -p 1 -m data/square01_quad.mesh -rs 3 -o -q -ra
mpirun -np 4 laghos -p 1 -m data/square_10x9_quad.mesh -rs 0 -ok 3 -ot
```

```
2 -s 7 -o -q -ra
```

run	step	dt	е	
1	1064	0.001578	50.3862948290	
2	952	0.000240	45.6800237914	

An implementation is considered valid if the final energy values are all within round-off distance from the above reference values.



## Performance Timing and FOM

Each time step in Laghos contains 3 major distinct computations:

- 1. The inversion of the global kinematic mass matrix (CG H1).
- 2. The force operator evaluation from degrees of freedom to quadrature points (Forces).
- 3. The physics kernel in quadrature points (UpdateQuadData).

By default, Laghos is instrumented to report the total execution times and rates, in terms of millions of degrees of freedom per second (megadofs), for each of these computational phases. These rates are reported as three separate figures of merits in the table below, together with a total combined execution rate which is the reportable **Figure of Merit (FOM)** for the benchmark:

node	s cores	order	Total dofs/node	FOM_1	FOM_2	FOM_3	FOM
1	36	Q3-Q2	119,468,548	184.054	341.243	170.887	190.272

These results were obtained with the following setup on the Quartz machine at LLNL with the gcc/8.1.0 and openmpi/4.0.0 modules. The vendor should provide a performance comparison to this run:

#### Contact

You can reach the Laghos team by emailing <u>laghos@llnl.gov</u> or by leaving a comment in the GitHub issue tracker.



High-Order Lagrangian Hydrodynamics Miniapp https://github.com/CEED/Laghos

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