

GridapDistributed: a massively parallel finite element toolbox in Julia

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Summary and statement of need

The ever-increasing demand for resolution and accuracy in mathematical models of physical processes governed by systems of Partial Differential Equations (PDEs) can only be addressed using fully-parallel advanced numerical discretization methods and scalable solution methods, thus able to exploit the vast amount of computational resources in state-of-the-art supercomputers. To this end, GridapDistributed is a registered Julia ([Bezanson et al., 2017](#)) software package which provides fully-parallel distributed memory data structures and associated methods for the Finite Element (FE) numerical solution of PDEs on parallel computers. Thus, it can be run on multi-core CPU desktop computers at small scales, as well as on HPC clusters and supercomputers at medium/large scales. The data structures in GridapDistributed are designed to mirror as far as possible their counterparts in the Gridap ([Badia & Verdugo, 2020](#)) Julia software package, while implementing/leveraging most of their abstract interfaces (see ([Verdugo & Badia, 2021](#)) for a detailed overview of the software design of Gridap). As a result, sequential Julia scripts written in the high-level Application Programming Interface (API) of Gridap can be used verbatim up to minor adjustments in a parallel distributed memory context using GridapDistributed. This equips end-users with a tool for the development of simulation codes able to solve real-world application problems on massively parallel supercomputers while using a highly expressive, compact syntax, that resembles mathematical notation. This is indeed one of the main advantages of GridapDistributed and a major design goal that we pursue.

In order to scale FE simulations to large core counts, the mesh used to discretize the computational domain on which the PDE is posed must be partitioned (distributed) among the parallel tasks such that each of these only holds a local portion of the global mesh. The same requirement applies to the rest of data structures in the FE simulation pipeline, i.e., FE space, linear system, solvers, data output, etc. The local portion of each task is composed by a set of cells that it owns, i.e., the *local cells* of the task, and a set of off-processor cells (owned by remote processors) which are in touch with its local cells, i.e., the *ghost cells* of the task ([Badia et al., 2020](#)). This overlapped mesh partition is used by GridapDistributed, among others, to exchange data among nearest neighbors, and to glue together global Degrees of Freedom (DoFs) which are sitting on the interface among subdomains. Following this design principle, GridapDistributed provides scalable parallel data structures and associated methods for simple grid handling (in particular, Cartesian-like meshes of arbitrary-dimensional, topologically n-cube domains), FE spaces setup, and distributed linear system assembly. It is in our future plans to provide highly scalable linear and nonlinear solvers tailored for the FE discretization of PDEs (e.g., linear and nonlinear matrix-free geometric multigrid and domain decomposition preconditioners). In the meantime, however, GridapDistributed can be combined with other Julia packages in order to realize the full potential required in real-world applications. These packages and their relation with GridapDistributed are overviewed in the next section.

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44 Building blocks and composability

45 [Figure 1](#) depicts the relation among GridapDistributed and other packages in the Julia pack-
 46 age ecosystem. The interaction of GridapDistributed and its dependencies is mainly designed
 47 with separation of concerns in mind towards high composability and modularity. On the one
 48 hand, Gridap provides a rich set of abstract types/interfaces suitable for the FE solution of
 49 PDEs (see ([Verdugo & Badia, 2021](#)) for more details). It also provides realizations (imple-
 50 mentations) of these abstractions tailored to serial/multi-threaded computing environments.
 51 GridapDistributed **implements** these abstractions for parallel distributed-memory computing
 52 environments. To this end, GridapDistributed also leverages (**uses**) the serial realizations
 53 in Gridap and associated methods to handle the local portion on each parallel task. (See
 54 [Figure 1](#) arrow labels.) On the other hand, GridapDistributed relies on PartitionedArrays
 55 ([Verdugo, 2021](#)) in order to handle the parallel execution model (e.g., message-passing via
 56 the Message Passing Interface (MPI) ([Message Passing Interface Forum, 2021](#))), global data
 57 distribution layout, and communication among tasks. PartitionedArrays also provides a paral-
 58 lel implementation of partitioned global linear systems (i.e., linear algebra vectors and sparse
 59 matrices) as needed in grid-based numerical simulations. While PartitionedArrays is an stand-
 60 alone package, segregated from GridapDistributed, it was designed with parallel FE packages
 61 such as GridapDistributed in mind. In any case, GridapDistributed is designed so that a dif-
 62 ferent distributed linear algebra library from PartitionedArrays might be used as well, as far
 63 as it is able to provide the same functionality.

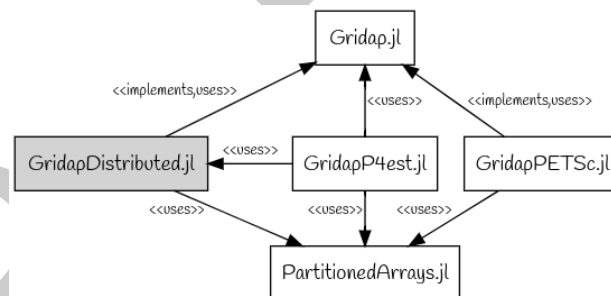


Figure 1: GridapDistributed and its relation to other packages in the Julia package ecosystem. In this diagram, each rectangle represents a Julia package, while the (directed) arrows represent relations (dependencies) among packages. Both the direction of the arrow and the label attached to the arrows are used to denote the nature of the relation. Thus, e.g., GridapDistributed depends on Gridap and PartitionedArrays, and GridapPETSc depends on Gridap and PartitionedArrays. Note that, in the diagram, the arrow direction is relevant, e.g., GridapP4est depends on GridapDistributed but not conversely.

64 As mentioned earlier, GridapDistributed offers a built-in Cartesian-like mesh generator, and
 65 does not provide, by now, built-in highly scalable solvers. To address this, as required by
 66 real-world applications, one can combine GridapDistributed with GridapP4est ([Martin, 2021](#))
 67 and GridapPETSc ([Verdugo et al., 2021](#)) (see [Figure 1](#)). The former provides a mesh data
 68 structure that leverages the p4est library as highly scalable mesh generation engine ([Burstedde
 69 et al., 2011](#)). This engine can mesh domains that can be expressed as a forest of adaptive
 70 octrees. The latter enables the usage of the highly scalable solvers (e.g., algebraic multigrid)
 71 in the PETSc library ([Balay et al., 2021](#)) to be combined with GridapDistributed.

72 Usage example

73 In order to confirm our previous claims on expressiveness, conciseness and productivity (e.g.,
 74 a very small number of lines of code), the example Julia script below illustrates how one

may use GridapDistributed in order to solve, in parallel, a 2D Poisson problem defined on the unit square. (In order to fully understand the code snippet, familiarity with the high level API of Gridap is assumed.) The domain is discretized using the parallel Cartesian-like mesh generator built-in in GridapDistributed. The only minimal burden posed on the programmer versus Gridap is a call to the `prun` function of PartitionedArrays right at the beginning of the program. With this function, the programmer sets up the PartitionedArrays communication backend (i.e., MPI communication backend in the example), specifies the number of parts and their layout (i.e., (2,2) 2D layout in the example), and provides a function (using Julia do-block syntax for function arguments in the example) to be run on each part. This function is equivalent to a sequential Gridap script, except for the `CartesianDiscreteModel` call, which, in GridapDistributed, also requires the `parts` argument passed back by the `prun` function. In a typical cluster environment, this example would be executed on 4 MPI tasks from a terminal as `mpirun -n 4 julia --project=. example.jl`.

```
using Gridap
using GridapDistributed
using PartitionedArrays
partition = (2,2)
prun(mpi,partition) do parts
    domain = (0,1,0,1)
    mesh_partition = (4,4)
    model = CartesianDiscreteModel(parts,domain,mesh_partition)
    order = 2
    u((x,y)) = (x+y)^order
    f(x) = -Δ(u,x)
    reffe = ReferenceFE(lagrangian,Float64,order)
    V = TestFESpace(model,reffe,dirichlet_tags="boundary")
    U = TrialFESpace(u,V)
    Ω = Triangulation(model)
    dΩ = Measure(Ω,2*order)
    a(u,v) = ∫( ∇(v)·∇(u) )dΩ
    l(v) = ∫( v*f )dΩ
    op = AffineFEOperator(a,l,U,V)
    uh = solve(op)
    writevtk(Ω,"results",cellfields=["uh"=>uh,"grad_uh"=>∇(uh)])
end
```

Parallel scaling benchmark

Figure 2 reports the strong (left) and weak scaling (right) of GridapDistributed when applied to an standard elliptic benchmark PDE problem, namely the 3D Poisson problem. In strong form this problem reads: find u such that $-\nabla \cdot (\kappa \nabla u) = f$ in $\Omega = [0,1]^3$, with $u = u_D$ on Γ_D (Dirichlet boundary) and $\partial_n u = g_N$ on Γ_N (Neumann Boundary); \mathbf{n} is the outward unit normal to Γ_N . The domain was discretized using the built-in Cartesian-like mesh generator in GridapDistributed. The code was run on the NCI@Gadi Australian supercomputer (3024 nodes, 2x 24-core Intel Xeon Scalable Cascade Lake cores and 192 GB of RAM per node) with Julia 1.7 and OpenMPI 4.1.2. For the strong scaling test, we used a fixed **global** problem size resulting from the trilinear FE discretization of the domain using a 300x300x300 hexaedra mesh (26.7 MDoFs) and we scaled the number of cores up to 21.9K cores. For the weak scaling test, we used a fixed **local** problem size of 32x32x32 hexaedra, and we scaled the number of cores up to 16.5K cores. A global problem size of 0.54 billion DoFs was solved for this number of cores. The reported wall clock time includes: (1) Mesh generation; (2) Generation of global FE space; (3) Assembly of distributed linear system; (4) Interpolation of a manufactured solution; (5) Computation of the residual (includes a matrix-vector product)

and its norm. Note that the linear solver time (GAMG built-in solver in PETSc) was not included in the total computation time as it is actually external to GridapDistributed.

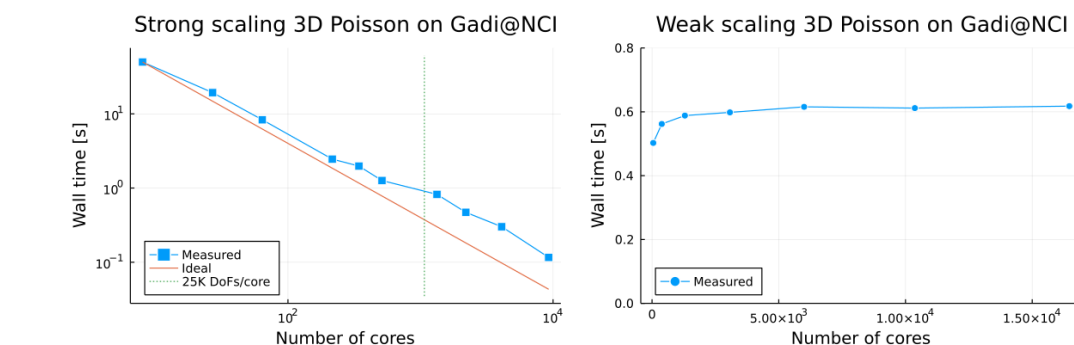


Figure 2: Strong (left) and weak (right) scaling of GridapDistributed when applied to 3D Poisson problem on the Australian Gadi@NCI supercomputer.

Figure 2 shows, on the one hand, an efficient reduction of computation times with increasing number of cores, even far beyond a relatively small load of 25K DoFs per CPU core. On the other hand, an asymptotically constant time-to-solution (i.e., perfect weak scaling) when the number of cores is increased in the same proportion of global problem size with a local problem size of $32 \times 32 \times 32$ trilinear FEs.

Demo application

To highlight the ability of GridapDistributed and associated packages (see Figure 1) to tackle real-world problems, and the potential behind its composable architecture, we consider a demo application with interest in the geophysical fluid dynamics community. This application solves the so-called non-linear rotating shallow water equations on the sphere, i.e., a surface PDE posed on a two-dimensional manifold immersed in three-dimensional space. This complex system of PDEs describes the dynamics of a single incompressible thin layer of constant density fluid with a free surface under rotational effects. It is often used as a test bed for horizontal discretisations with application to numerical weather prediction and ocean modelling. We in particular considered the synthetic benchmark proposed in (Galewsky et al., 2016), which is characterized by its ability to generate a complex and realistic flow.

For the geometrical discretization of the sphere, the software uses the so-called cubed sphere mesh (Ronchi et al., 1996), which was implemented using GridapP4est. The spatial discretization of the equations relies on GridapDistributed to build a **compatible** set of FE spaces (Gibson et al., 2019) for the system unknowns (fluid velocity, fluid depth, potential vorticity and mass flux) grounded on Raviart-Thomas and Lagrangian FEs defined on the manifold (Rognes et al., 2013). Compatible FEs are advanced discretization techniques that preserve at the discrete level physical properties of the continuous equations. The spatial discretization is stabilized using the so-called Anticipated Potential Vorticity Method (APVM) (Rognes et al., 2013). Time integration is based on a implicit trapezoidal rule, and thus a fully-coupled nonlinear problem has to be solved at each time step. In order to solve this nonlinear problem, we leveraged a Newton-GMRES solver preconditioned with an algebraic preconditioner provided by GridapPETSc (on top of PETSc 3.16). The *exact* Jacobian of the shallow water system was computed/assembled at each nonlinear iteration.

Figure 3 shows the magnitude of the vorticity field after 6.5 simulation days (left) and the results of a strong scaling study of the model on the Australian Gadi@NCI supercomputer (right). The reported times correspond to the *total* wall time of the first 10 time integration

steps; these were the only ones (out of 3600 time steps, i.e., 20 simulation days with a time step size of 480 secs.) that we could afford running for all points in the plot due to limited computational budget reasons. We considered two different problem sizes, corresponding to 256x256 and 512x512 quadrilaterals/panel cubed sphere meshes, resp. Overall, Figure 3 confirms a remarkable ability of the ecosystem of Julia packages at hand to efficiently reduce computation times with increasing number of CPU cores for a complex, real-world computational model.

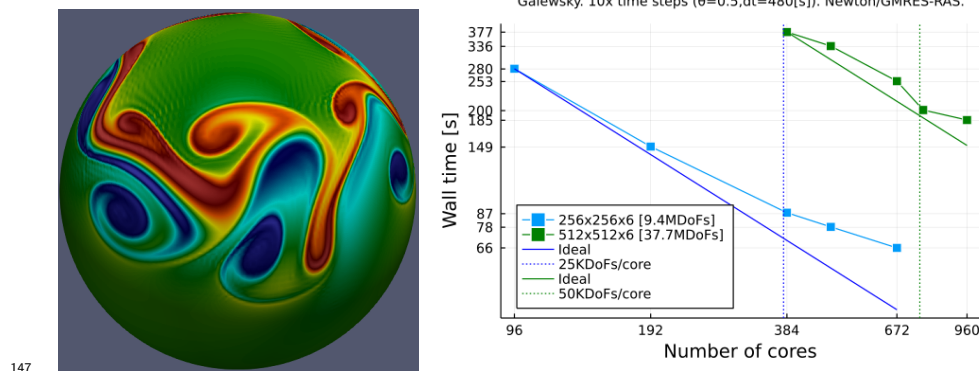


Figure 3: Magnitude of the vorticity field after 6.5 simulation days with a coarser 48x48 quadrilaterals/panel cubed sphere mesh (left) and strong scaling (right) of the non-linear rotating shallow water equations solver on the Australian Gadi@NCI supercomputer.

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