Controlling Parallel CFD Simulations in Julia from C/Fortran with `libtrixi`

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What is it all about?

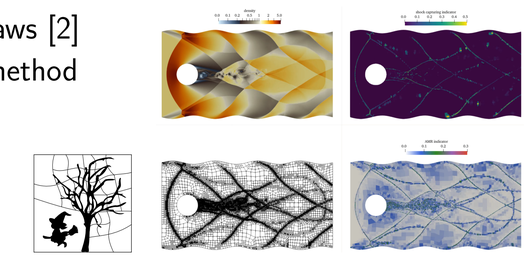
- Enhance legacy applications with modern programming concepts
- Keep original C/C++/Fortran code
- Add new features written in a high-level, user-friendly language
- Do not sacrifice performance
- Support heterogeneous HPC environments

Why Julia?

- Modern high-level programming language
- Lots of ready-to-use packages
- Dynamic typing, rapid prototyping capability
- Just-in-time compilation
- Solves two-language problem: easy to use and performant, HPC-ready

Who is that `Trixi.jl`?

- Numerical simulation framework for conservation laws [2]
- Adaptive high-order discontinuous Galerkin (DG) method
- Entropy stable and entropy conserving fluxes
- Focus: extensibility, usability, performance
- ∼20 main developers, ∼75k lines of code
- Performance on par with classical codes [3]



Who would possibly be using this?

- `MESSy`, the *Modular Earth Submodel System*, written in Fortran
- Project *ADAPTEX* (BMBF call *SCALEXA*):
  Adaptive Earth system modelling with strongly reduced computation time for exascale-supercomputers
- `Trixi.jl` as an alternative dynamical core, i. e. computational fluid dynamics (CFD) solver
- Makes `MESSy` exascale-ready, allows `MESSy` to leverage Julia's vendor-agnostic GPU support

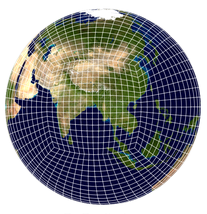
Can Fortran speak Julia?

Introduce `libtrixi`:

- `LibTrixi.jl`: Julia interface to `Trixi.jl`
- C API to `LibTrixi.jl`
- Fortran wrapper for C API

Does it work?

- Simulation of a baroclinic instability [1]
- Cubed sphere discretization of earth's atmosphere
- 3D compressible Euler equations
- Controlled from Fortran main program
- 98 304 mesh cells, 6^3 degrees of freedom each
- Computed on 6144 MPI ranks



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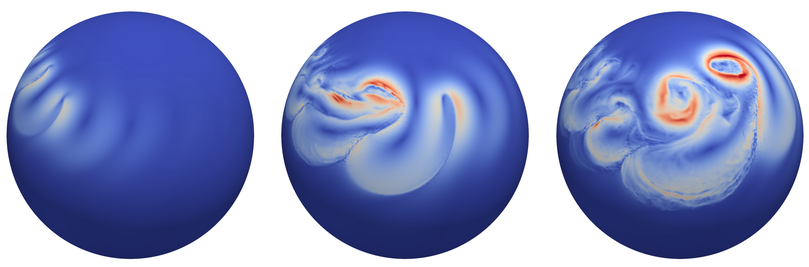
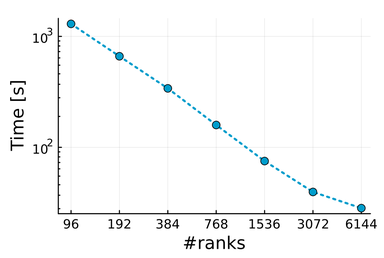


Velocity magnitude near surface after about 7.5, 10 and 12 days



Strong scaling (1h simulated time)

How fast is it?

- Benchmarks: 2D Sedov blast wave, 3D baroclinic instability (compressible Euler equations)
- Minimum runtime in seconds from 5 runs
- Negligible overhead for practical applications!

	`Trixi.jl`	`LibTrixi.jl`	`libtrixi`	
			classic	`PackageCompiler.jl`
2D	7.9	11.3	11.2	11.1
3D	327.0	332.0	329.0	334.0

How to use it?

- Build and install `libtrixi` using `cmake`
- Set up Julia runtime environment (`libtrixi` comes with a script!)
- Alternative: `PackageCompiler.jl`, skips C API, no runtime required
- Configure simulation through code (*elixir*)

```julia
using Trixi, LibTrixi
function init_simstate()
  equations = CompressibleEulerEquations2D(gamma = 1.4)
  solver = DGSEM(polydeg = 3, surface_flux = flux_lax_friedrichs)
  mesh = P4estMesh((8, 8), (-1.0, -1.0), (1.0, 1.0), polydeg = 3)
  my_init(x, t, equations) = ...
  semi = SemidiscretizationHyperbolic(mesh, equations, my_init, solver)
  ...
  # OrdinaryDiffEq
  integrator = init(ode, ...)
  return SimulationState(semi, integrator)
end
```

- Include header/module, link `libtrixi.so`, run

```
program trixi_controller_simple_f
  use LibTrixi
  ...
  ! Initialize Trixi
  call trixi_initialize(julia_runtime_dir)
  ! Set up the Trixi simulation
  handle = trixi_initialize_simulation(elixir)
  do
    if ( trixi_is_finished(handle) ) exit
    call trixi_step(handle)
  end do
  ! Finalize Trixi simulation
  call trixi_finalize_simulation(handle)
  ! Finalize Trixi
  call trixi_finalize()
end program
```

- Handle (integer) to address multiple simulations

How is it done?

- Fortran API: thin wrapper around C code

```
interface
  integer(c_int) function trixi_nelements(handle) bind(c)
    integer(c_int), value, intent(in) :: handle
  end function
end interface
```

- C API: Obtain, store, and call Julia function pointers
- Uses Julia C API

```c
int trixi_nelements(int handle) {
  const char* command = "@cfunction(trixi_nelements, Cint, (Cint,))";
  jl_value_t* res = jl_eval_string(command);
  int (*nelements)(int) = (void *) jl_unbox_voidpointer(res);
  return nelements(handle);
}
```

- Julia API: Get simulation state, call `Trixi.jl` function
- Retrieves non-integral Julia data

```julia
Base.@ccallable function trixi_nelements(simstate_handle::Cint)::Cint
    simstate = load_simstate(simstate_handle)
    _, _, solver, cache = mesh_equations_solver_cache(simstate.semi)
    return nelements(solver, cache)
end
```

What else?

Reproducibility

repository `libtrixi` `Trixi.jl` *ADAPTEX* `MESSy`

[1] C. Jablonowski and D. Williamson. "A baroclinic instability test case for atmospheric model dynamical cores". *Q. J. R. Meteorol. Soc.* (2006). DOI: https://doi.org/10.1256/qj.06.12.

[2] M. Schlottke-Lakemper et al. *Trixi.jl: Adaptive high-order numerical simulations of hyperbolic PDEs in Julia*. https://github.com/trixi-framework/Trixi.jl. 2020.

[3] H. Ranocha et al. "Efficient Implementation of Modern Entropy Stable and Kinetic Energy Preserving Discontinuous Galerkin Methods for Conservation Laws". *ACM Trans. Math. Softw.* (2023). DOI: 10.1145/3625559.

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