# Gridap: Towards productivity and performance in Julia

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My concerns about **poor productivity wrt software development** 

#### Workflow

Design new method  $\rightarrow$  analyse it  $\rightarrow$  implement it (rapid prototyping)  $\rightarrow$  exploit it in (large scale) applications (performance)

Probably not your case: Focused on analysis (academic examples) or application side (existing libraries OK)

## Scientific computing teams

PhD students (3-4y), postdocs (1-3y), no computer scientists

#### Software dev policies

Start from scratch: Academic codes in dynamic languages (MATLAB, Python...), wasting previous work, no performance, usually not accessible code (no reproducible science)

## **Existing numerical PDE libraries**

#### Software dev policies

**Reuse:** Excellent pool of high-performance libraries: deal.ii, Fenics, FEMPAR, MOOSE, libmesh, Firedrake, DUNE, NGSolve, etc.

- Static languages (C++, FORTRAN08...) for performance
- Excellent if they provide all you need (Python interfaces)
- Far more involved if not (productivity loss)

## **Productivity vs performance**

#### **Productivity**

Related to **dynamic languages** (Python, MATLAB...): More expressive, no compilation step, interactive development (debugging on-the-fly), better for math-related bugs (no benefit from static compilation), no set-up of environment (compilers, system libraries, etc)

#### **Performance**

Related to **static languages** (C/C++,FORTRAN,...): Compilers generate *highly optimised* code



https://julialang.org/

21st century FORTRAN, designed for numerical computation (MIT, 2011-)

All-in-one (?)

**Productive:** Dynamic language (as Python, MATLAB...)

Performant: Advanced type-inference system +

just-in-time (JIT) compilation

- Not OO: No inheritance of concrete types (only abstract types), use composition, not inheritance, classify by their actions, not their attributes...
- Multiple dispatching paradigm: functions not bound to types, dispatching wrt all arguments

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Let us play a little with with Julia...

Gridap seed started in Christmas 2018 trying to increase productivity in my team

Some key decisions based on previous experience and Julia capabilities:

- Functional-like style i.e. immutable objects, no state diagram (just cache arrays for performance)
- Lazy evaluation of expressions (implement unary/binary expression trees for types)

In the spirit of the lazy matrix example...

#### CellField

Given a *cell* in a partition  $\mathcal{T}$  of a manifold  $\mathcal{M}$  (e.g. cells, faces, edges in a mesh), it provides a Field. A Field assigns a *physical quantity (n-tensor) per space(-time)* point in the manifold.

Key method, lazy evaluation: Given an array of points per cell in  $\mathcal{T}$ , we can evaluate a CellField, returning an array of scalars/vectors/tensors (FieldValue) per cell per point

```
Evaluate(cf::CellField,ps::CellPoints)
::CellArray{FieldValue}
```

## FEs, Integration, assembly

We also implement operations:

- Unary operations: e.g.  $\nabla()$ ,  $\nabla \times ()$ ,  $\nabla \cdot ()$ , etc.
- Binary operations: inner(, ), ×, etc.

With these types, we represent *FE functions, FE bases, constitutive models, etc.* 

Applying a CellField to a CellPoints (integration points) plus expression trees we can integrate forms and assemble matrices

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Let us look at Gridap Tutorial 1

## **Gridap status**

Gridap is pretty comprehensive (big thanks to F Verdugo's amazing work at UPC):

- Lagrangian, Raviart-Thomas, Nedelec, dG
- Multifield or multiphysics methods
- Interaction with GMesh, Pardiso, PETSc...
- dimension-agnostic (5-dim Laplacian), order-agnostic

Quite rich documentation, tutorials, automatic testing, etc.

After 1 year and two developers (part time!)... highly productive environment

Objective: same software for research and teaching

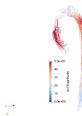
 Designing FE tutorials in MTH5321 - Methods of computational mathematics

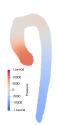
## **Gridap for teaching**

#### Objective: same software for research and teaching

 One undergrad AMSI project on Gridap (Connor Mallon, Monash): No idea about FEs/coding → from patient-specific MRI data of aorta velocity field to pressure field (Navier-Stokes solver...) in about 2 months







## **Gridap future**

#### This is just the beginning:

- Distributed-memory integration/assembly
- Parallel hp-adaptivity
- Historic variables in nonlinear constitutive models
- Virtual element methods
- Space-time discretisations
- Interaction with other Julia packages (optimisation, ML, UQ, ODE, automatic diff...)
- ...

#### Performance analysis:

- Poisson solver w/ 1st order FEs on 145<sup>3</sup> mesh in 30 sec (CG+AMG about 60%), similar for 30<sup>4</sup> mesh
- Trying to write performant code (type stable), but NO optimisation yet
- Performance analysis on the way (x2-3 performance hit OK if x2-3 productivity, but does not seem to be the case)
- Further topic: In fact, type stability + JIT compilation eliminates virtualisation overhead in static languages

Learning Julia

julialang.org

Gridap

github.com/gridap/Gridap.jl

Gridap tutorials

github.com/gridap/Tutorials

## **Further reading**

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## Thanks!