

How simple should using Ferrite.jl get?

Knut Andreas Meyer

Complete FE program for solving the nonlinear, time-dependent problem

$$c(u)\dot{u} - [k \nabla u] \cdot \nabla = h, \quad c(u) = c_0 + au$$

```
using Ferrite, FESolvers, FerriteProblems, FerriteAssembly, FerriteViz, CairoMakie
import FerriteAssembly.ExampleElements: WeakForm
grid = generate_grid(Quadrilateral, (10,10)); dΩ = union(getfaceset.((grid,), ("left","top"))...)
ip = Lagrange{RefQuadrilateral,1}()
dh = close!(add!(DofHandler(grid), :u, ip))
ch = close!(add!(ConstraintHandler(dh), Dirichlet(:u, dΩ, Returns(0.0))));
cv = CellValues(QuadratureRule{RefQuadrilateral}(2), ip)
material = WeakForm((δu, ∇δu, u, ∇u, u_dot, _) -> δu*((1+10u)*u_dot - 1) + (∇δu · ∇u))
problem = FerriteProblem(FEDefinition(DomainSpec(dh, material, cv); ch))
solver = QuasiStaticSolver(;nlsolver=NewtonSolver(), timestepper=FixedTimeStepper(;num_steps=10, Δt=0.1))
solve_problem!(problem, solver)
FerriteViz.solutionplot(dh, FESolvers.getunknowns(problem))
```

Introduction

FE program for solving the nonlinear, time-dependent problem

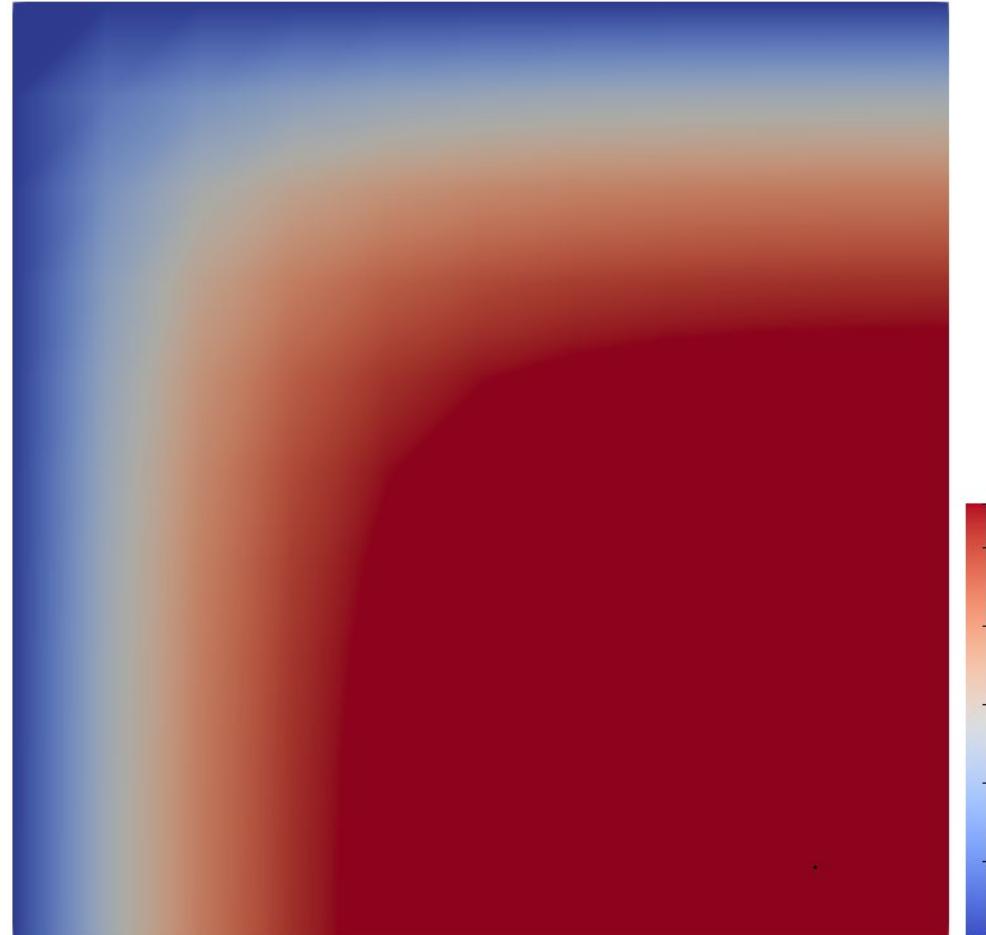
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problem = FerriteProblem(FEDefinition(DomainSpec(dh, material, cv); ch))
solver = QuasiStaticSolver(;nlsolver=NewtonSolver(), timestepper=FixedTimeStepper(;num_steps=10, Δt=0.1))
solve_problem!(problem, solver)
FerriteViz.solutionplot(dh, FESolvers.getunknowns(problem))
```

```
using Ferrite, FerriteViz

function setup()
    grid = generate_grid(Quadrilateral, (10,10)); dΩ =
union(getfaceset.((grid,), ("left","top"))...)
    ip = Lagrange{RefQuadrilateral,1}()
    dh = close!(add!(DofHandler(grid), :u, ip))
    ch = close!(add!(ConstraintHandler(dh), Dirichlet(:u, dΩ, Returns(0.0))))
    cv = CellValues(QuadratureRule{RefQuadrilateral}(2), ip)
    return dh, ch, cv
end

function element_routine!(Ke, re, ae, ae_old, Δt, cv)
    for q_point in 1:getquadpoints(cv)
        dΩ = getdetdΩ(cv, q_point)
        u = function_value(cv, q_point, ae)
        uold = function_value(cv, q_point, ae_old)
        ∇u = function_gradient(cv, q_point, ae)
        udot = (u-uold)/Δt
        re += Ke * (u - uold) - re
        ae += ∇u · udot - ae
    end
    return re, ae
end
```



Introduction

Complete FE program for solving the nonlinear, time-dependent weak form

$$c(u)\dot{u} - [k \nabla u] \cdot \nabla = h, \quad c(u) = c_0 + au$$

```
# Ferrite.jl syntax
grid = generate_grid(Quadrilateral, (10,10)); dΩ = union(getfaceset.((grid,), ("left","top"))...)
ip = Lagrange{RefQuadrilateral,1}()
dh = close!(add!(DofHandler(grid), :u, ip))
ch = close!(add!(ConstraintHandler(dh), Dirichlet(:u, dΩ, Returns(0.0))));
cv = CellValues(QuadratureRule{RefQuadrilateral}(2), ip)

# FerriteAssembly.jl
material = WeakForm((δu, ∇δu, u, ∇u, u_dot, args...) -> δu*((1+10u)*u_dot - 1) + 1.0*(∇δu · ∇u))
domainspec = DomainSpec(dh, material, cv)

# FerriteProblems.jl
problem = FerriteProblem(FEDefinition(domainspec; ch))

# FESolvers.jl
solver = QuasiStaticSolver(;nlsolver=NewtonSolver(), timestepper=FixedTimeStepper(;num_steps=10, Δt=0.1))
solve_problem!(problem, solver)

# FerriteViz.jl
FerriteViz.solutionplot(dh, FESolvers.getunknowns(problem))
```

Outline

- **Introduction to the “Ecosystem” built on top of Ferrite.jl**
 - FerriteAssembly.jl
 - FESolvers.jl
 - FerriteProblems.jl
- **Examples from research and fun**
 - Multi-field problems: Frost damage in concrete
 - Highly nonlinear problems: Partially saturated porous media
 - Phase-field damage with [@lijas’s IGA.jl](#)
- **Conclusions and outlook**
 - Challenges in the design
 - When to use?

FerriteAssembly.jl

```
work!(worker,
```

```
    domainbuffer; a, aold)
```

Current and old
degrees of freedom

What

- Assembler
- Integrator

Where

- Cell domain
- Face domain
- Interface domain

User to define:

```
# Assemble: Cell domain
element_routine!(Ke, re, cell_state, ae, material, cellvalues, cellbuffer)
element_residual!(re, cell_state, ae, material, cellvalues, cellbuffer)

# Assemble: Face domain
face_routine!(Ke, re, ae, material, facevalues, facebuffer)
face_residual!(re, ae, material, facevalues, facebuffer)

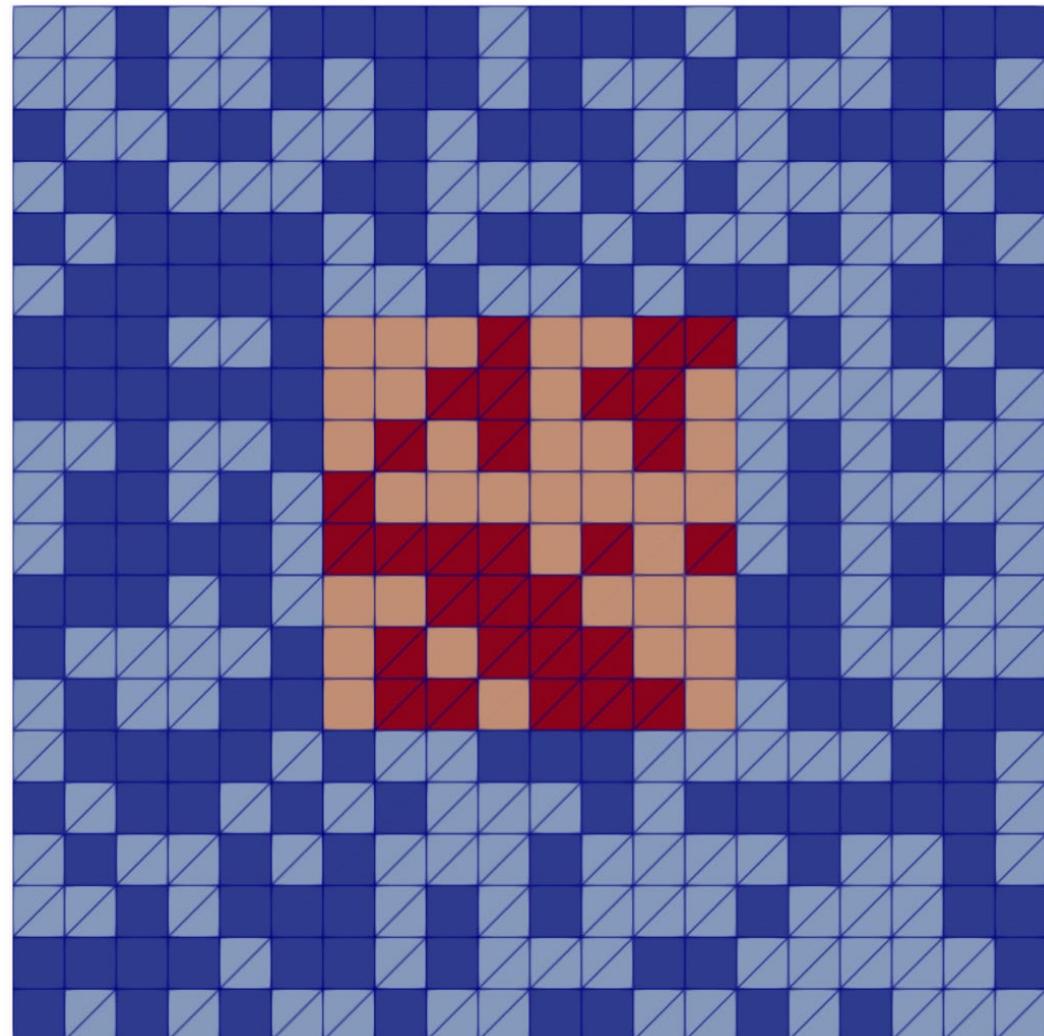
# Integrate: Cell and face domain
integrate_cell!(val, cell_state, ae, material, cv, cellbuffer)
integrate_face!(val, ae, material, cv, facebuffer)
```

FerriteAssembly.jl

What constitutes a domain?

- Same SubDofHandler
 - Same fields
 - Same interpolations
 - Same cell type
- Same FEValues
 - Same quadrature rule
- Same “material” type (i.e. same weak form)

- Inclusion (tet) `sdh_tet, inclusion_material`
- Inclusion (quad) `sdh_quad, inclusion_material`
- Matrix (tet) `sdh_tet, matrix_material`
- Matrix (quad) `sdh_quad, matrix_material`



FerriteAssembly.jl

How is a domain defined?

```
# Create single DomainSpec
ds = DomainSpec(sdh::[Sub]DofHandler, material, fe_values; [set], [user_data],
                 kwargs...)

# Create single domain buffer
domainbuffer = setup_domainbuffer(ds; kwargs...)
```

```
struct DomainBuffer{I,B,S,SDH<:SubDofHandler}
    set::Vector{I}
    itembuffer::B
    states::Dict{Int,S} # Indexed by cellid
    old_states::Dict{Int,S}
    sdh::SDH
end
```

```
face_residual!(re, ae, material,
               facevalues, facebuffer)
```

```
element_routine!(Ke, re, cell_state, ae, material, cellvalues, cellbuffer)
```

FerriteAssembly.jl

How to define buffers for multiple domains?

```
# Create single DomainSpec
ds = DomainSpec(sdh::[Sub]DofHandler, material, fe_values; [set], [user_data],
                 kwargs...)

# Create single domain buffer
domainbuffer = setup_domainbuffer(ds; kwargs...)

# Create multiple domain buffers
domainbuffers = setup_domainbuffers(Dict(
    "domain 1"=>DomainSpec(...),
    "domain 2"=>DomainSpec(...));
    kwargs...)
```

DomainBuffer -> Dict{String, <:DomainBuffer}

FerriteAssembly.jl

How to make things multithreaded?

```
# Create single DomainSpec
ds = DomainSpec(sdh::[Sub]DofHandler, material, fe_values; [set], [user_data],
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domainbuffer = setup_domainbuffer(ds; kwargs...)

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    kwargs...)
```

DomainBuffer -> Dict{String, <:DomainBuffer}

FerriteAssembly.jl

How to make things multithreaded?

```
# Create single DomainSpec
ds = DomainSpec(sdh::[Sub]DofHandler, material, fe_values; [set], [user_data],
                 kwargs...)

# Create single domain buffer
domainbuffer = setup_domainbuffer(ds; threading=true, kwargs...)

# Create multiple domain buffers
domainbuffers = setup_domainbuffers(Dict(
    "domain 1"=>DomainSpec(...),
    "domain 2"=>DomainSpec(...));
    threading=true, kwargs...)
```

DomainBuffer -> ThreadedDomainBuffer

Dict{String, <:DomainBuffer} -> Dict{String, <:ThreadedDomainBuffer}

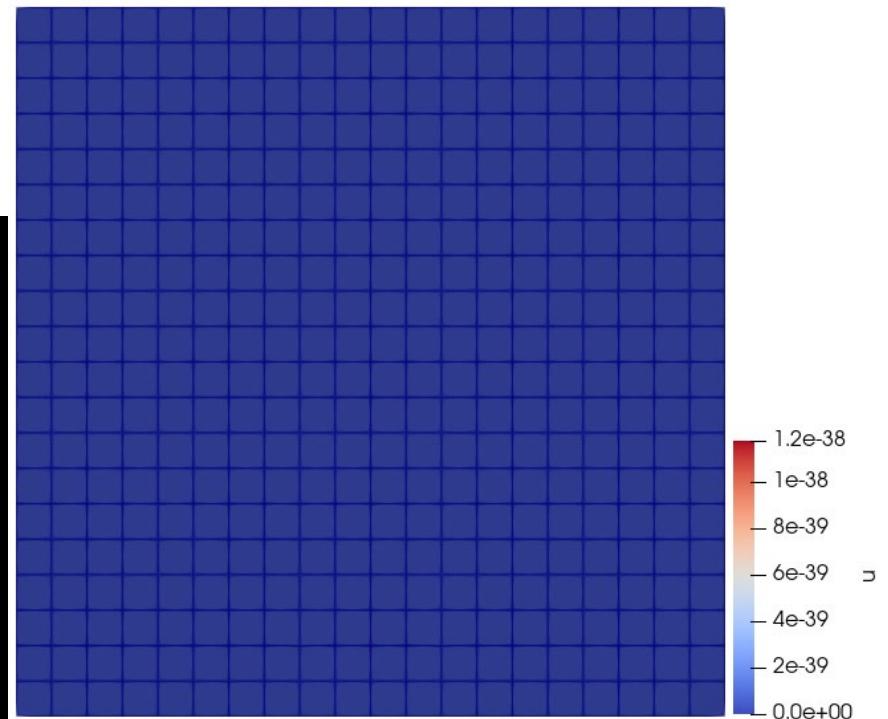
FerriteAssembly.jl

Let's do some work!

```
using Ferrite, FerriteAssembly
import FerriteAssembly.ExampleElements: StationaryFourier
# Ferrite.jl setup
grid = generate_grid(Quadrilateral, (20, 20));
dΩ = union(getfaceset.((grid), ("left", "top", "bottom", "right"))...)
ip = Lagrange{RefQuadrilateral,1}()
dh = close!(add!(DofHandler(grid), :u, ip))
ch = close!(add!(ConstraintHandler(dh), Dirichlet(:u, dΩ, Returns(0.0))));
cv = CellValues(QuadratureRule{RefQuadrilateral}(2), ip)
K = create_sparsity_pattern(dh)
a, r = [zeros(ndofs(dh)) for _ in 1:2]

# FerriteAssembly.jl
material = StationaryFourier(#=k=#1.0)
domainbuffer = setup_domainbuffer(DomainSpec(dh, material, cv))
assembler = start_assemble(K, r)
work!(assembler, domainbuffer; a=a)

apply!(K, r, ch)
a .-= K\r
```

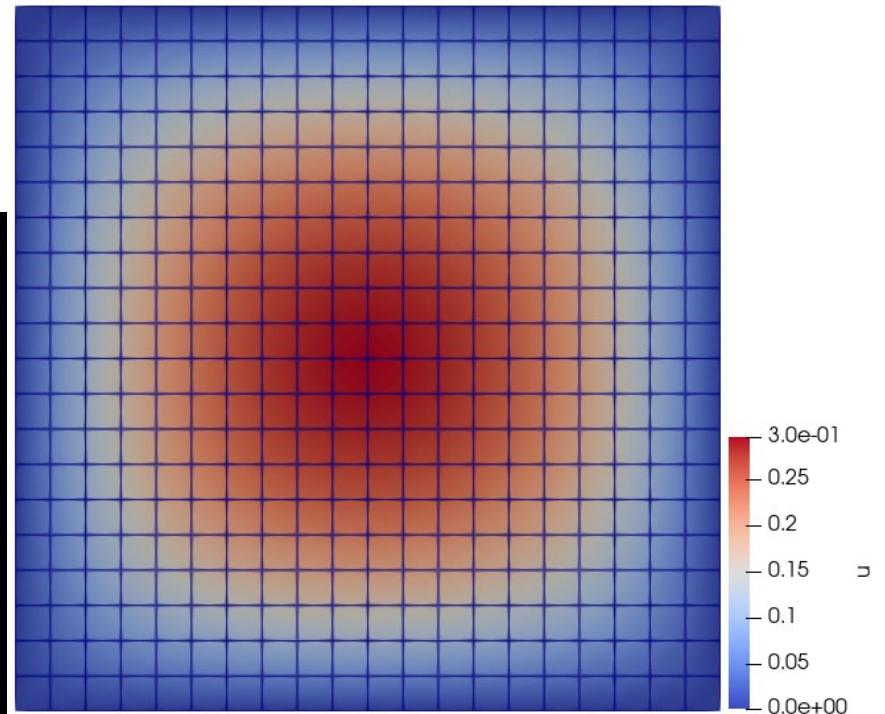


FerriteAssembly.jl

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# FerriteAssembly.jl
material = StationaryFourier(#=k=#1.0)
domainbuffer = setup_domainbuffer(DomainSpec(dh, material, cv))
assembler = start_assemble(K, r)
work!(assembler, domainbuffer; a=a)
lh = LoadHandler(dh)
add!(lh, BodyLoad(:u, #=qr_order=# 2, Returns(-1.0)))
apply!(r, lh, 0.0)
apply!(K, r, ch)
a .-= K\r
```



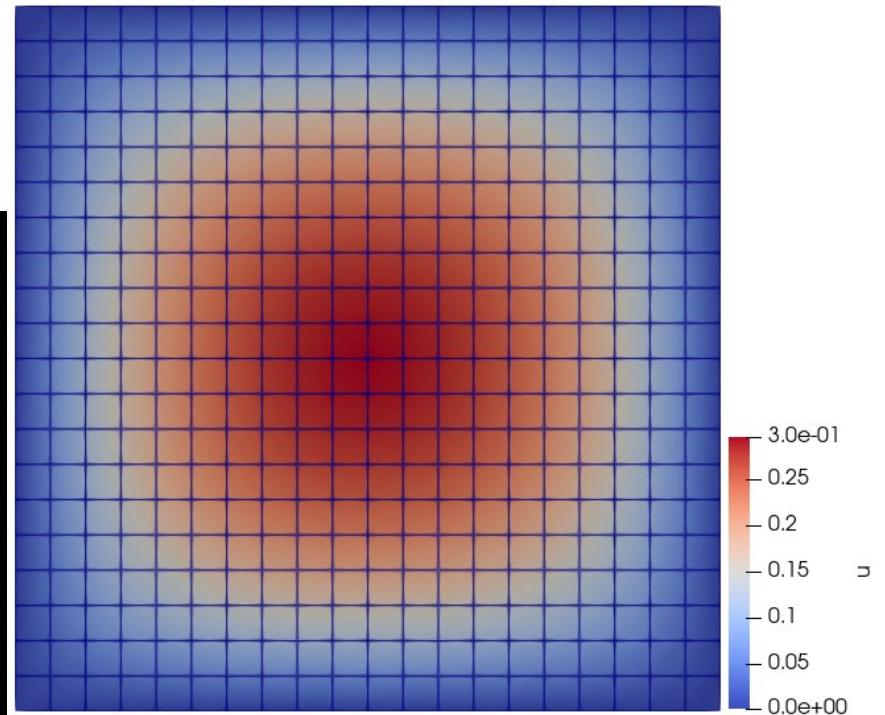
FerriteAssembly.jl

Not only for assembling

```
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import FerriteAssembly.ExampleElements: StationaryFourier
# Ferrite.jl setup
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# FerriteAssembly.jl
material = StationaryFourier(#=k=#1.0)
domainbuffer = setup_domainbuffer(DomainSpec(dh, material, cv))
assembler = start_assemble(K, r)
work!(assembler, domainbuffer; a=a)
lh = LoadHandler(dh)
add!(lh, BodyLoad(:u, #=qr_order=# 2, Returns(-1.0)))
apply!(r, lh, 0.0)
apply!(K, r, ch)
a .-= K\r
```

$$\text{Average temperature, } \bar{T} = \frac{\int_{\Omega} T \, d\Omega}{\int_{\Omega} 1 \, d\Omega}$$



```
integrator = SimpleIntegrator((u, ∇u, s)->(1, u),
                                #=initial_value=(0.0, 0.0))
work!(integrator, domainbuffer; a=a)
area = integrator.val[1]
average_temperature = integrator.val[2]/area
@show average_temperature
average_temperature = 0.14005406375299906
```

FerriteAssembly.jl

Fast automatic differentiation

```
# Assemble: Cell domain  
element_residual!(re, state, ae, material, cellvalues, cellbuffer)
```

```
Assemble 100x100 heat equation
```

```
Standard AD:           11.371 ms (60000 allocations: 9.16 MiB)  
Analytical tangent:    4.609 ms (    0 allocations: 0 bytes)  
Special buffer for AD: 4.721 ms (    0 allocations: 0 bytes)
```

```
# Create single domain buffer  
domainbuffer = setup_domainbuffer(ds; autodiffbuffer=true,  
kwargs...)
```

FerriteAssembly.jl

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Heat Equation

Viscoelasticity with state variables

Multiple fields

Multiple materials

How-to

Threaded assembly

Automatic differentiation

Local constraint application

Robin boundary conditions

Volume integration

Surface integration

Reference

Summary of FerriteAssembly.jl

1. Define your "material" type
2. Define your low-level routine
`element_routine!, face_residual!, integrate_cell!, etc.`
3. Standard Ferrite.jl setup, dh, ch, fe_values, etc.
4. `db = setup_domainbuffer(DomainSpec(...); kwargs...)`
5. `worker = start_assemble(...) # (for example)`
6. `work!(worker, db; kwargs....)`

```
assembler = KeReAssembler(K, r; ch, apply_zero=true)
```

FESolvers.jl

Your problem – your way

Define your problem type

```
struct MyProblem{...}  
    ...  
end  
problem = MyProblem(...)
```

Overload a set of functions from FESolvers, e.g.

```
FESolvers.update_problem!(problem, Δx, update_spec)  
FESolvers.getjacobian(problem)  
FESolvers.postprocess!(problem, step, solver)
```

Define time stepper and nonlinear solver

```
solver = QuasiStaticSolver(;  
    nlsolver=NewtonSolver(),  
    timestepper=FixedTimeStepper(;num_steps=10, Δt=0.1))
```

Solve the problem

```
solve_problem!(problem, solver)
```

FerriteProblems.jl

*A Ferrite.jl problem for FESolvers.jl
- building on FerriteAssembly.jl*

```
# Ferrite.jl syntax
grid = generate_grid(Quadrilateral, (10,10)); dΩ = union(getfaceset.((grid,), ("left","top"))...)
ip = Lagrange{RefQuadrilateral,1}()
dh = close!(add!(DofHandler(grid), :u, ip))
ch = close!(add!(ConstraintHandler(dh), Dirichlet(:u, dΩ, Returns(0.0))));
cv = CellValues(QuadratureRule{RefQuadrilateral}(2), ip)

# FerriteAssembly.jl
material = WeakForm((δu, ∇δu, u, ∇u, u_dot, args...) -> δu*((1+10u)*u_dot - 1) + 1.0*(∇δu · ∇u))
domainspec = DomainSpec(dh, material, cv)

# FerriteProblems.jl
problem = FerriteProblem(FEDefinition(domainspec; ch))

# FESolvers.jl
solver = QuasiStaticSolver(;nlsolver=NewtonSolver(), timestepper=FixedTimeStepper(;num_steps=10, Δt=0.1))
solve_problem!(problem, solver)
```

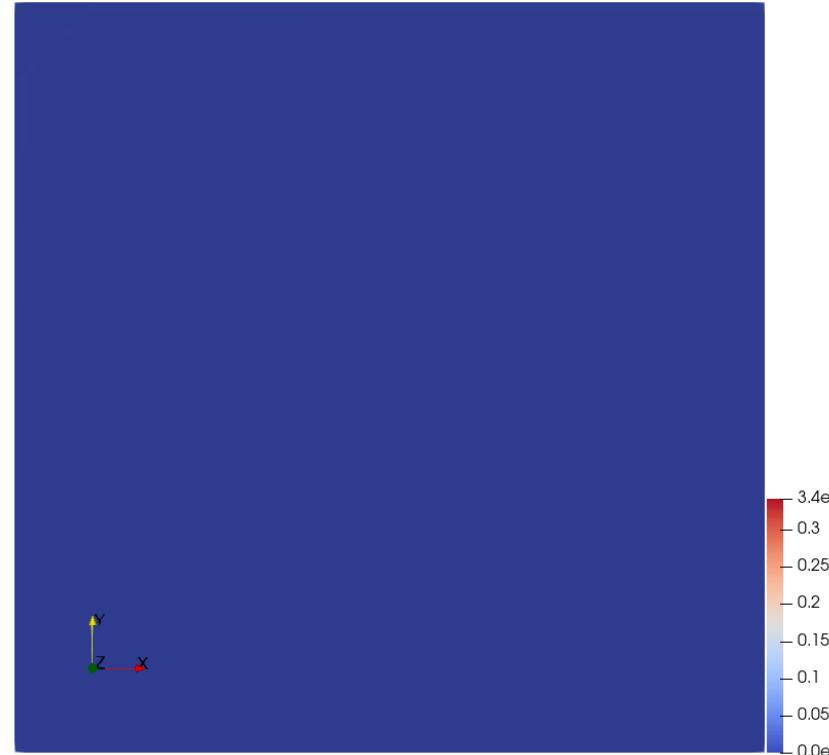
FerriteProblems.jl

A *Ferrite.jl* problem for *FESolvers.jl*

```
@kwdef struct NLHeatPostProc{PVD}
    pvd::PVD=paraview_collection("solution")
end
function FESolvers.postprocess!(post::NLHeatPostProc, problem, st)
    dh = FerriteProblems.get_dofhandler(problem)
    vtk_grid(string("solution", step), dh) do vtk
        vtk_point_data(vtk, dh, FESolvers.getunknowns(problem))
        post.pvd[FerriteProblems.get_time(problem)] = vtk
    end
end
function FerriteProblems.close_postprocessing(post::NLHeatPostProc, problem)
    vtk_save(post.pvd)
end

problem = FerriteProblem(FEDefinition(domainspec; ch), NLHeatPostProc())

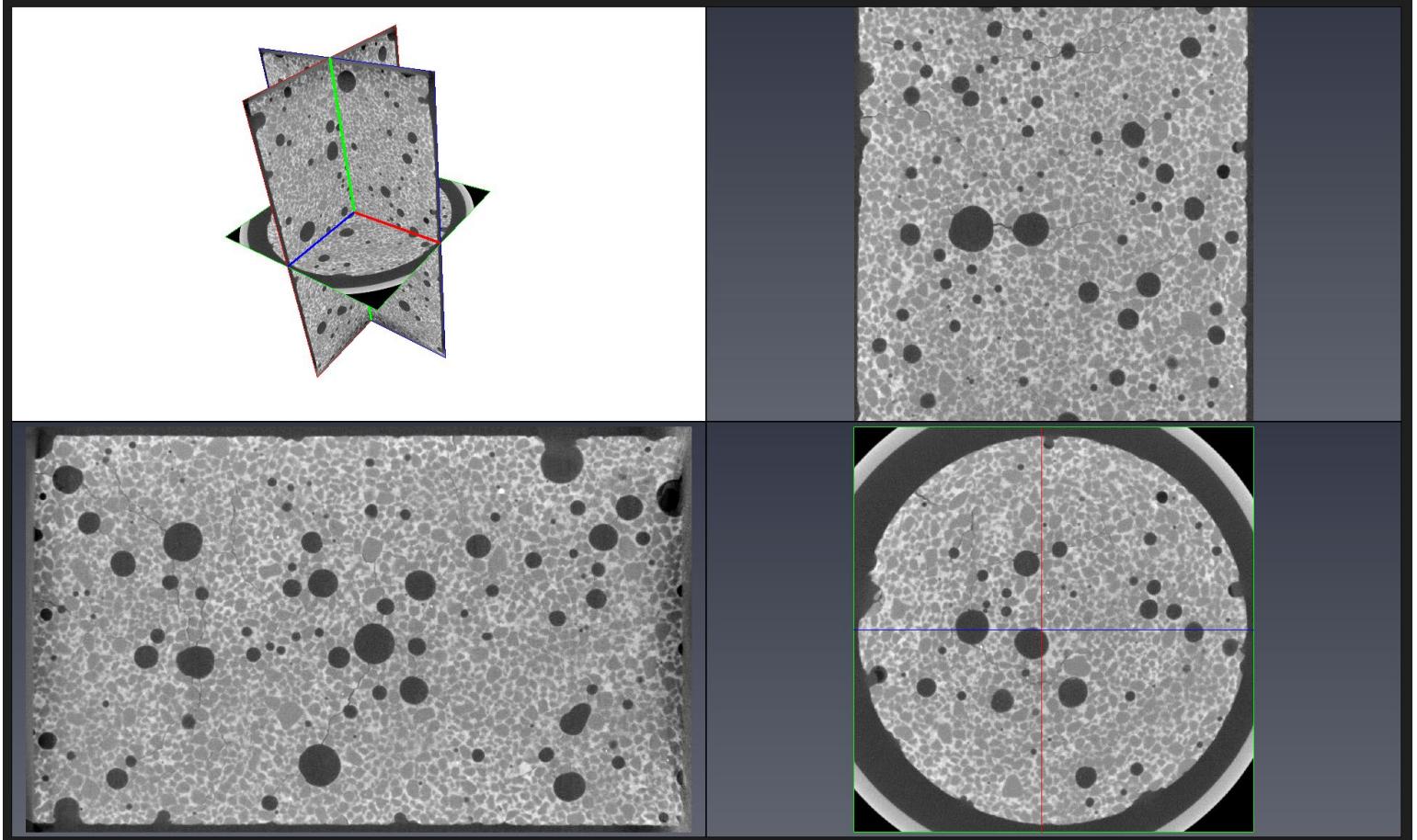
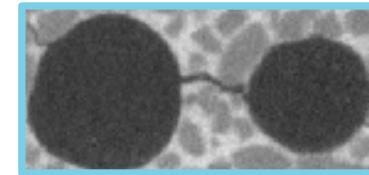
solver = QuasiStaticSolver(;nlsolver=NewtonSolver(),
                           timestepper=FixedTimeStepper(;num_steps=10, Δt=0.1))
solve_problem!(problem, solver)
```



Examples

From research and fun

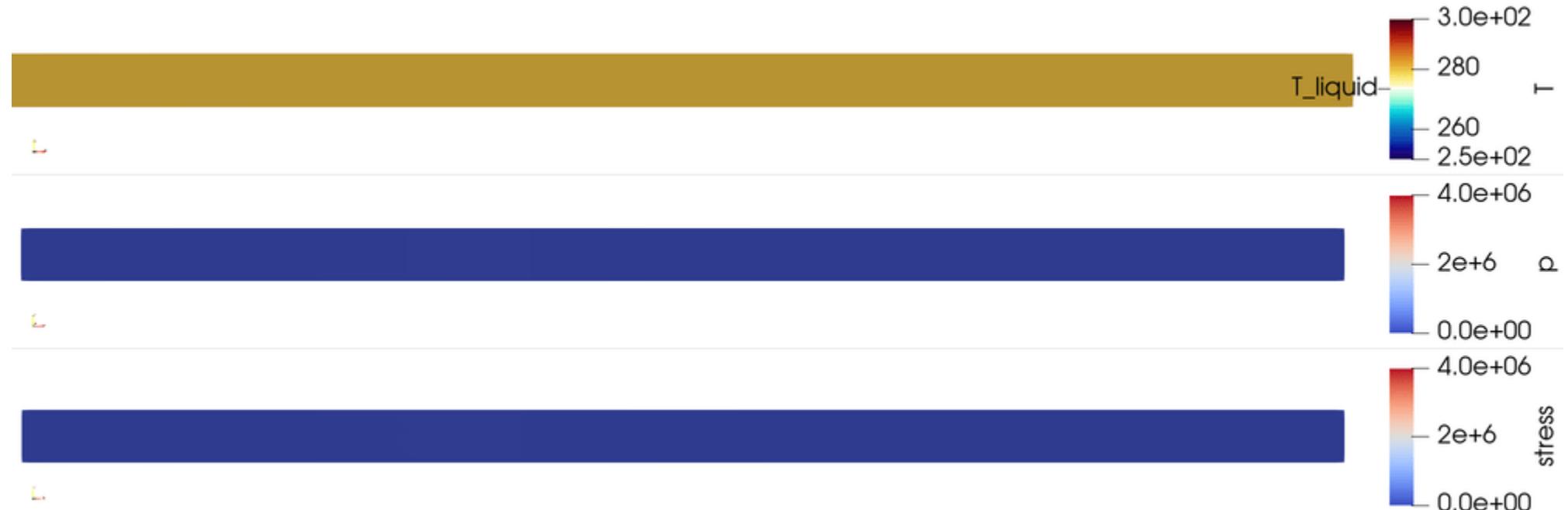
Frost damage in concrete



Credit
Aykut Levent
Roland Kruse (IAM)

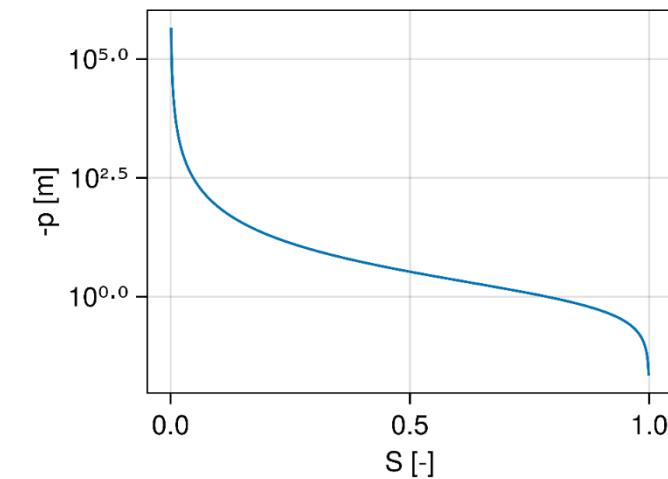
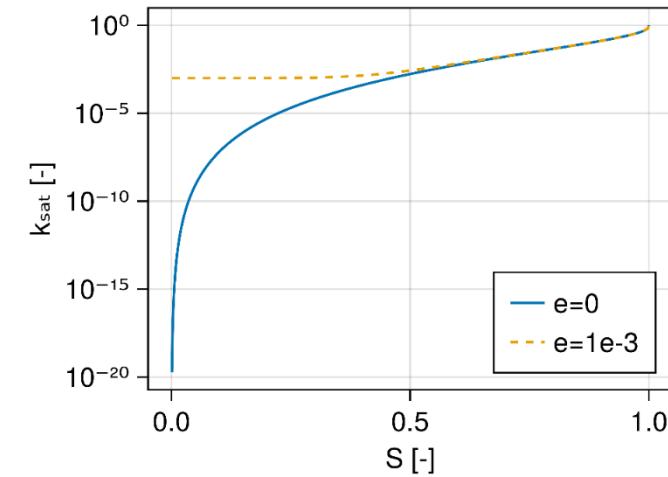
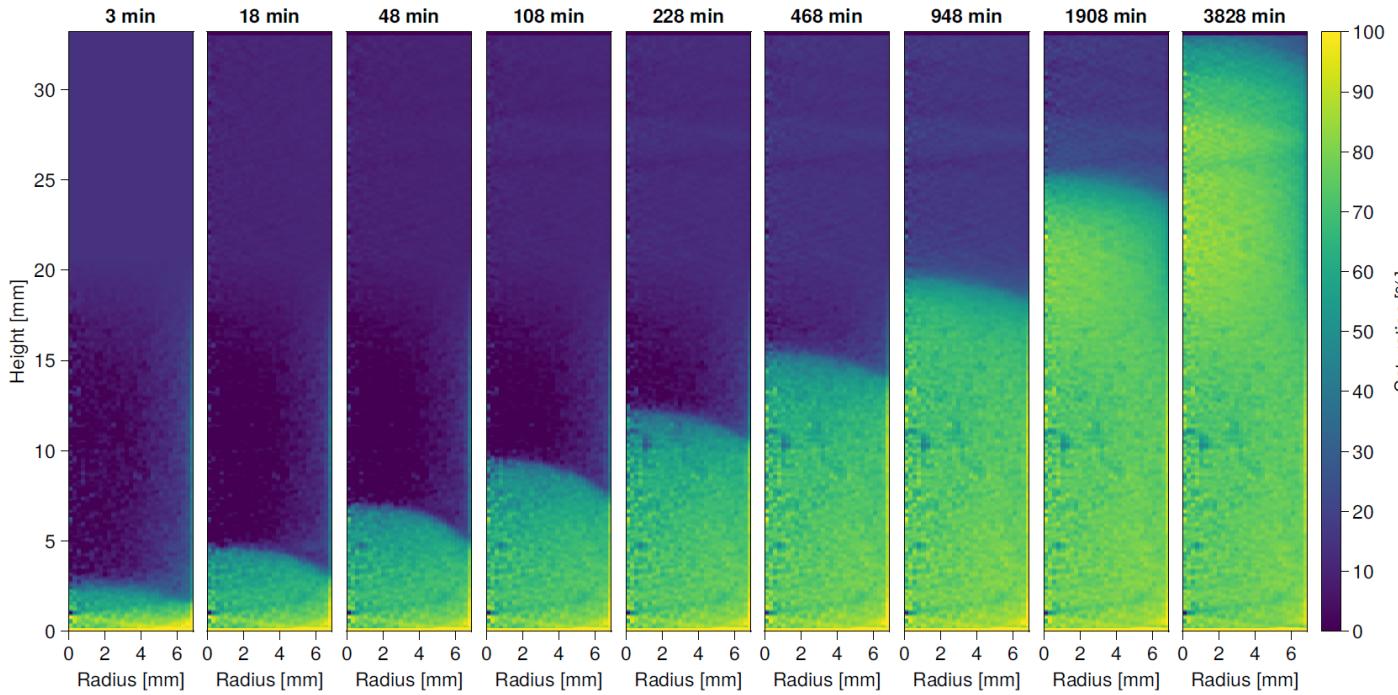
Frost damage in concrete

- Mechanical equilibrium (linear elasticity)
 - Mass conseration (darcy flow)
 - Energy balance (Fick's law)
- + Phase transformation: Freezing/thawing
-> Volume expansion



Highly nonlinear problems

Partially saturated porous media



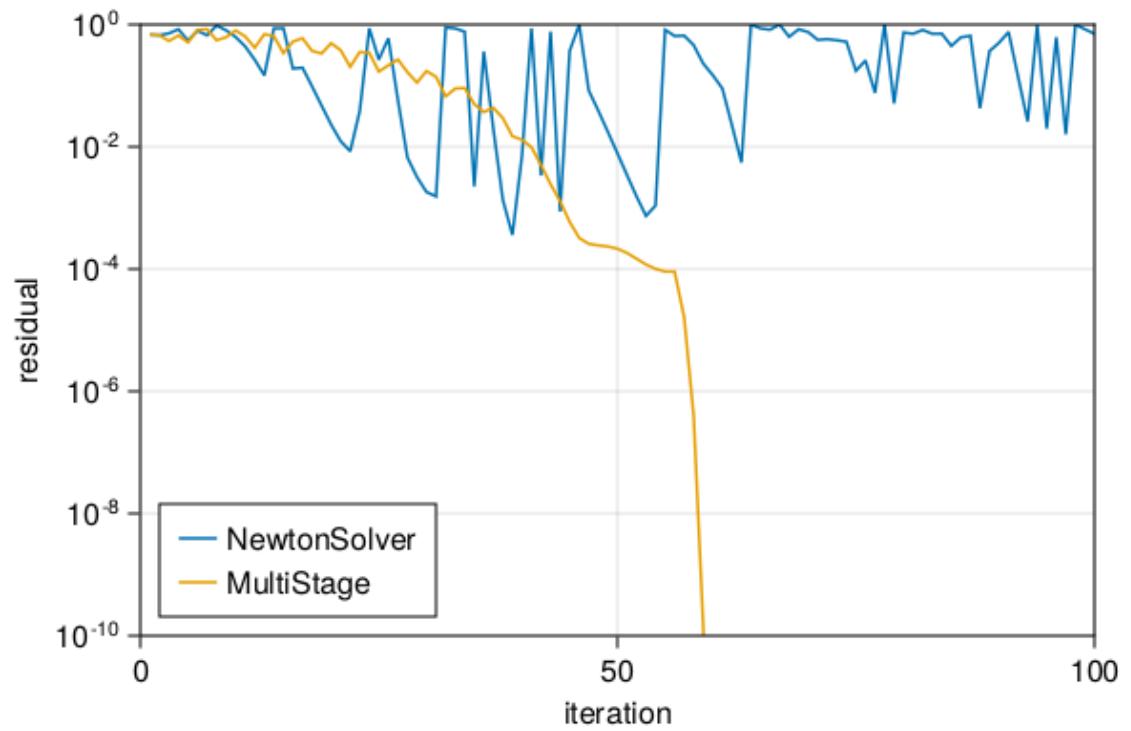
Highly nonlinear problems

```
import PorousMedia: JacobianSpec

# Fast, but requires good guess!
newton_solver = NewtonSolver();
    linsolver=ITU.TridiagonalSolver(),
    tolerance=1.e-10, maxiter=100,
    update_type=JacobianSpec(:TrueJacobian))

# Slow, but less sensitive to guess!
picard_solver = NewtonSolver();
    linsolver=ITU.TridiagonalSolver(),
    tolerance=1.e-04, maxiter=100,
    update_type=JacobianSpec(:ModifiedPicard))

# Best of both worlds?
FESolvers.MultiStageSolver([
    picard_solver, newton_solver]
    false)
```



Phase-field fracture with IGA.jl

- For fun
- Simulate brittle fracture
- Phase-field model from Bharali et al. (2023)
- Combine FerriteAssembly/FerriteProblems etc. with @ljias' IGA.jl
- Simulate fracture of “plate with a hole”

```
# Create the grid using routines in IGA.jl
grid = create_mesh();

# Define the special IGA-interpolation
ip = BernsteinBasis{2,(2,2)}()
qr = QuadratureRule{2,RefCube}(4) # As usual

# Define the special IGA cell values
cv = (
    u = BezierCellValues(CellVectorValues(qr, ip)),
    d = BezierCellValues(CellScalarValues(qr, ip)))

dh = ... # Create [Mixed]DofHandler as usual
ch = ... # Create ConstraintHandler as usual

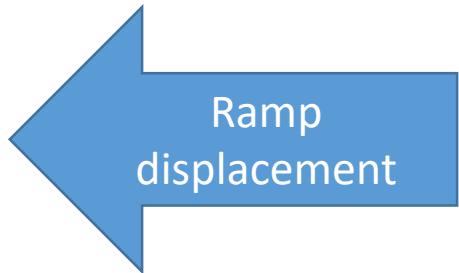
# DomainSpec and FEDefinition as usual
domain_spec = DomainSpec(sdh, material, cv)
def = FEDefinition(domain_spec; ch)

# Define problem and solve it as usual
problem = FerriteProblem(def, post)
solve_problem!(problem, solver)
```

R. Bharali, F. Larsson, and R. Jänicke, “A micromorphic phase-field model for brittle and quasi-brittle fracture,” *Comput. Mech.*, 2023, doi: 10.1007/s00466-023-02380-1.

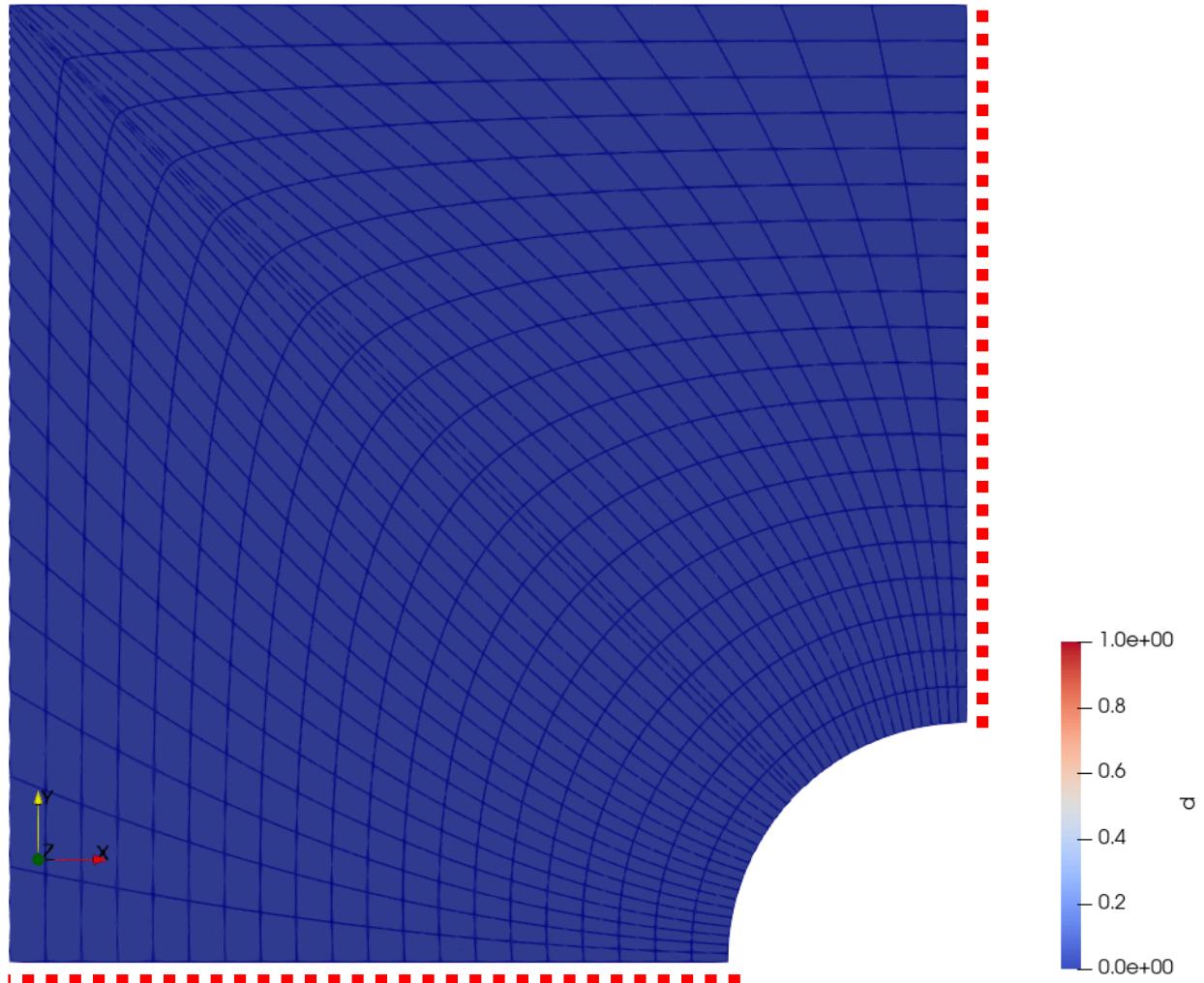
Phase-field fracture with IGA.jl

- Simulate brittle fracture
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- Combine FerriteAssembly/FerriteProblems etc. with @ljias' IGA.jl
- Simulate fracture of “plate with a hole”



▪▪▪ Symmetry conditions

R. Bharali, F. Larsson, and R. Jänicke, “A micromorphic phase-field model for brittle and quasi-brittle fracture,” *Comput. Mech.*, 2023, doi: 10.1007/s00466-023-02380-1.



Challenges and outlook

Challenges

When there is a bug in a user's element routine

```
struct MyMat end

FerriteAssembly.create_cell_state(::MyMat, cv::CellValues, args...) = zeros(getnquadpoints(cv))

function FerriteAssembly.element_residual!(re, state, ae, ::MyMat, cv, buffer)
    old_state = FerriteAssembly.get_old_state(buffer)
    for q_point in 1:getnquadpoints(cv)
        dΩ = getdetJdV(cv, q_point)
        ∇u = function_gradient(cv, q_point, ae)
        e = old_state[q_point] + ∇u·∇u # Calculate accumulated "energy"
        for i in 1:getnbasisfunctions(cv)
            ∇δu = shape_gradient(cv, q_point, i)
            re[i] += (∇δu · ∇u) *(1 + e)*dΩ
        end
        state[q_point] = e
    end
end
```

state::Vector{Float64}
e::ForwardDiff.Dual

state[q_point] = ForwardDiff.value(e)

Challenges

When there is a bug in a user's element routine

1/6 of the error message....

```
If the following error is related to converting objects with `ForwardDiff.Dual`'s
entries into objects with regular numbers, please consult the docs of `element_residual!`  

ERROR: MethodError: no method matching Float64(::ForwardDiff.Dual{ForwardDiff.Tag{FerriteAs
Nothing}, Float64, Vec{2, Float64}, Vec{2, Float64}, Float64, Vec{2, Float64}, QuadratureRu
FerriteAssembly.CellBuffer{Float64, Vector{Vec{2,
Float64}}}, CellValues{Lagrange{RefQuadrilateral, 1, Nothing}, Float64, Vec{2, Float64}, Vec
Lagrange{RefQuadrilateral, 1, Nothing}}, NamedTuple{(:u,), Tuple{UnitRange{Int64}}}}, MyMat,
```

Closest candidates are:

(`::Type{T}`) (`::Real`, `::RoundingMode`) where `T<:AbstractFloat`

```
SparseArrays.SparseMatrixCSC{Float64, Int64}, Vector{Float64}, FerriteAssembly.DomainBuffer{Int64, FerriteAssembly.CellBuffer{Float64, VecCellValues{Lagrange{RefQuadrilateral, 1, Nothing}, Float64, Vec{2, Float64}, Vec{2, Float64}, Float64, Vec{2, Float64}, QuadratureRule{RefLagrange{RefQuadrilateral, 1, Nothing}}, NamedTuple{(:u,), Tuple{UnitRange{Int64}}}, MyMat, Vector{Float64}, Nothing, Nothing}, Vector{Float64, Grid{2, Quadrilateral, Float64}}}}, FerriteProblems.TolScaling{FerriteProblems.AbsoluteResidual, FerriteAssembly.NoScaling, Nothing}}, Nothing; :QuasistaticSolver{NewtonSolver{BackslashSolver, NoLineSearch, Float64}, FixedTimeStepper{Float64}})
@ FESolvers C:\Users\meyer\.julia\packages\FESolvers\7W19R\src\FESolvers.jl:43
[21] top-level scope
@ C:\Users\meyer\Presentations\2023\FerriteCon\Code\Example4\error.jl:35
```

Challenges

When the problem is not converging

Using FerriteAssembly you can

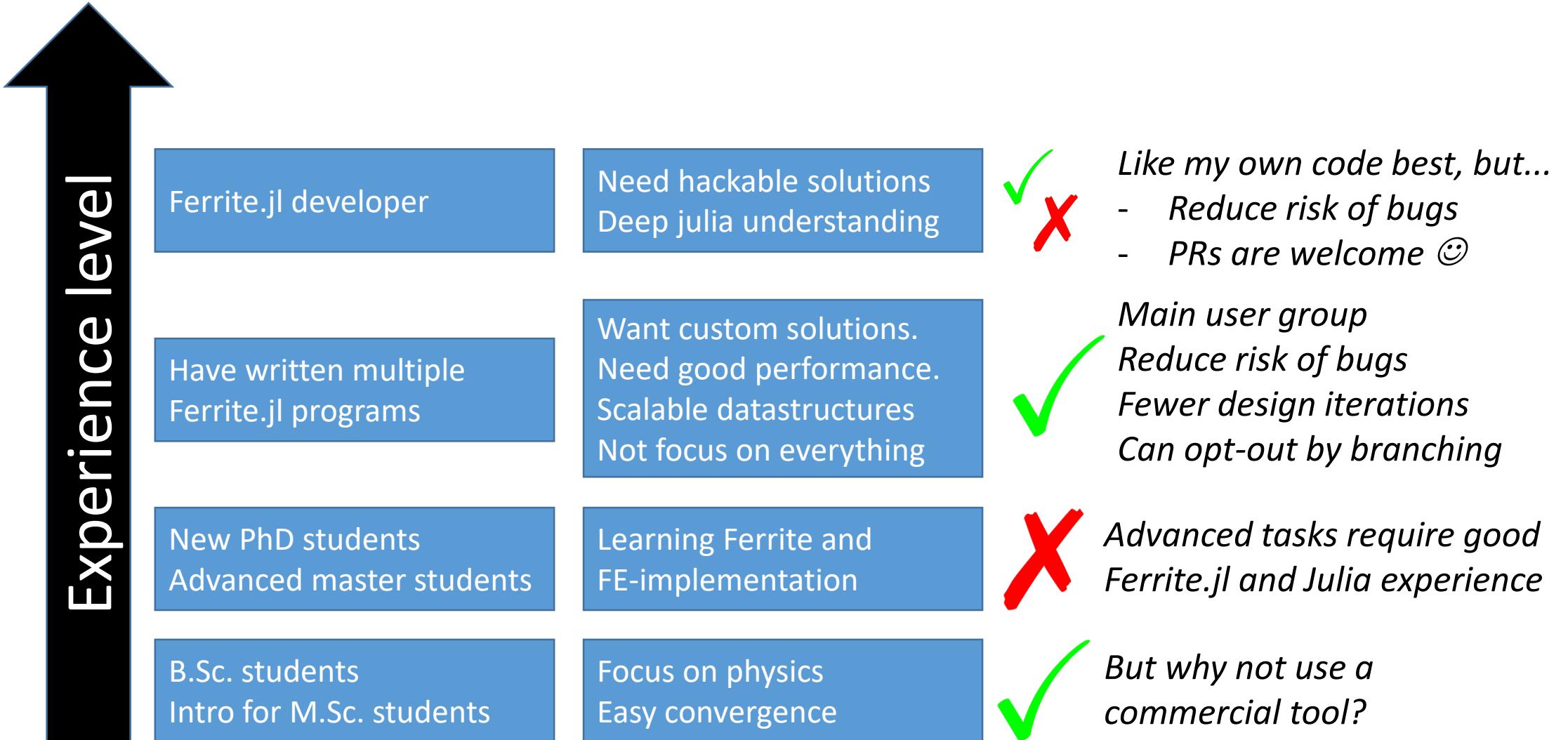
- 1) Use relative residual tolerance for each field, based on the L_p-norm of nodal “force” contributions

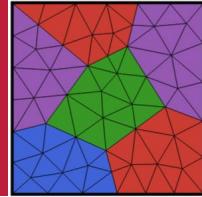
Using FESolvers you can

- 1) Use the adaptive time stepper
(Based on @lijas' algorithm)
- 2) Use linesearches (by @koehlerson)
- 3) Use improved initial guess strategies (under development)
- 4) Implement quasi-Newton iterations and even adaptively switching between different methods
(under development)
- 5) Implement your custom nonlinear solver

Before you cross this line, you probably want to step through the code in FESolvers and FerriteProblems

To use or not to use





Final remarks

FerriteAssembly.jl: Perform work on domains efficiently

github.com/knutam/FerriteAssembly.jl

FESolvers.jl: Solve nonlinear [quasi]time-dependent problems

github.com/knutam/FESolvers.jl

FerriteProblems.jl: Defines a problem to be solved with FESolvers.jl

github.com/knutam/FerriteProblems.jl

- **FerriteAssembly.jl**
 - A package like this can benefit the Ferrite.jl community by
 - Defining a common interface for defining physics – easy to share code
 - Remove a lot of boilerplate for “boring” coding, e.g. postprocessing
 - Call for feedback: Check it out and let me know of any dealbreakers!
- **FESolvers.jl and FerriteProblems.jl**
 - Difficult to make it general, hackable, and easy to use
 - Currently: Good for benchmarking and checking your own code
 - Not possible, nor the aim, to compete with commercial codes