Solving the Partitioned Heat Equation Using FEniCS and preCICE

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Department of Informatics
Chair of Scientific Computing

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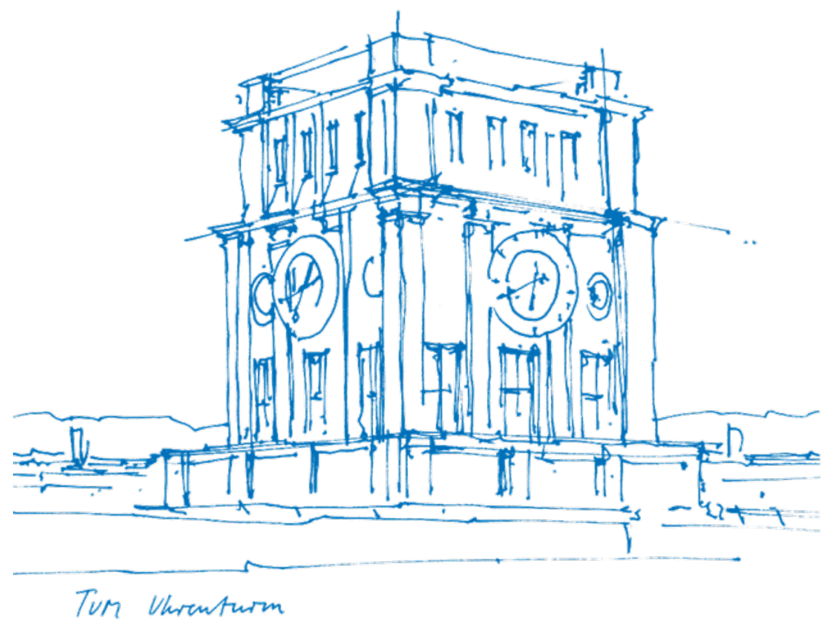
Mathematics (Faculty of Sciences)
Numerical Analysis



Siegen, Germany
November 29, 2018

Agenda

Partitioned Approach

Heat Equation with FEniCS

Coupling with preCICE

Results

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A few Disclaimers:

This talk is **not**

- a talk about FEM
- a talk about coupling algorithms
- a talk with proper mathematical notation

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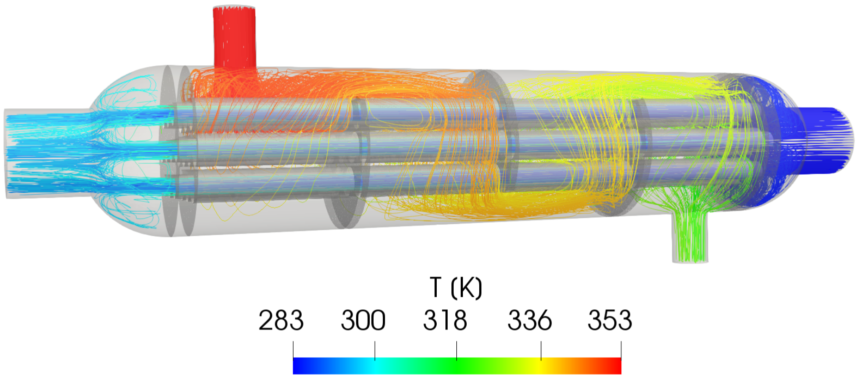
I will talk about

- software
- the partitioned approach
- where you can find my code
- how you can use my code

Partitioned Approach

Coupled problems

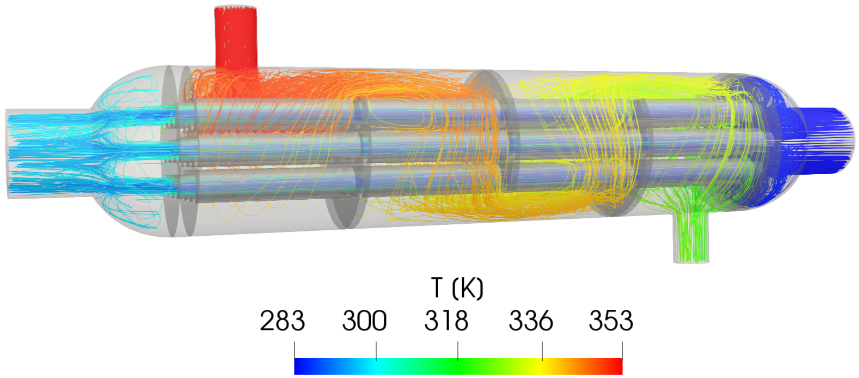


shell and tube heat exchanger using OpenFOAM and CalculiX[1]

[1] Figure from *Rusch, A., Uekermann, B. Comparing OpenFOAM's Intrinsic Conjugate Heat Transfer Solver with preCICE-Coupled Simulations. Technical Report, 2018.*

Partitioned Approach

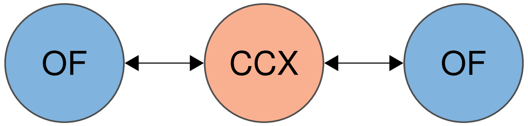
Coupled problems



shell and tube heat exchanger using OpenFOAM and CalculiX[1]

Basic idea:

- reuse existing solvers
- combine single-physics to solve multi-physics
- only exchange "black-box" information



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Partitioned Approach

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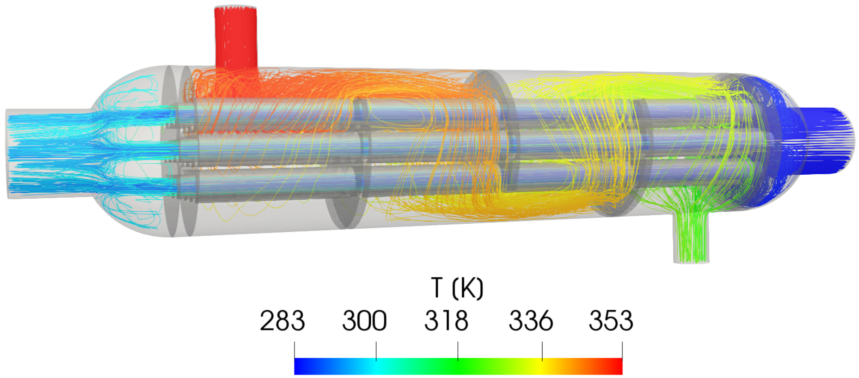

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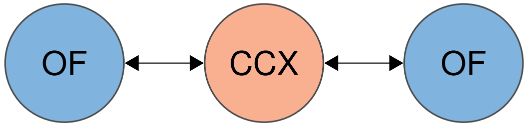

What we do today:

- couple with preCICE library
- use FEniCS as a solver for toy problem

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Partitioned Approach

preCICE[1]

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Features

- communication
- coupling schemes
- mapping
- time interpolation
- **official adapters** for OpenFOAM, SU2,...

preCICE

github.com/precice

---

[1] *Bungartz, H.-J., et al. (2016). preCICE – A fully parallel library for multi-physics surface coupling.*
[2] *Uekermann, B., et al. (2017). Official preCICE Adapters for Standard Open-Source Solvers.*

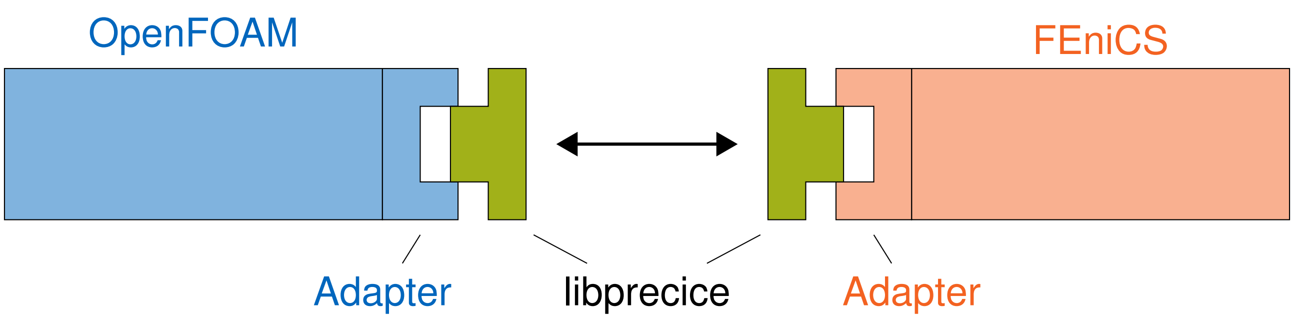
Partitioned Approach

preCICE[1]

Adapter[2]

- access preCICE API
- isolated layer between solver and preCICE
- support component exchangeability
- don't change existing (reliable, well-tested) code

github.com/precice



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Partitioned Approach

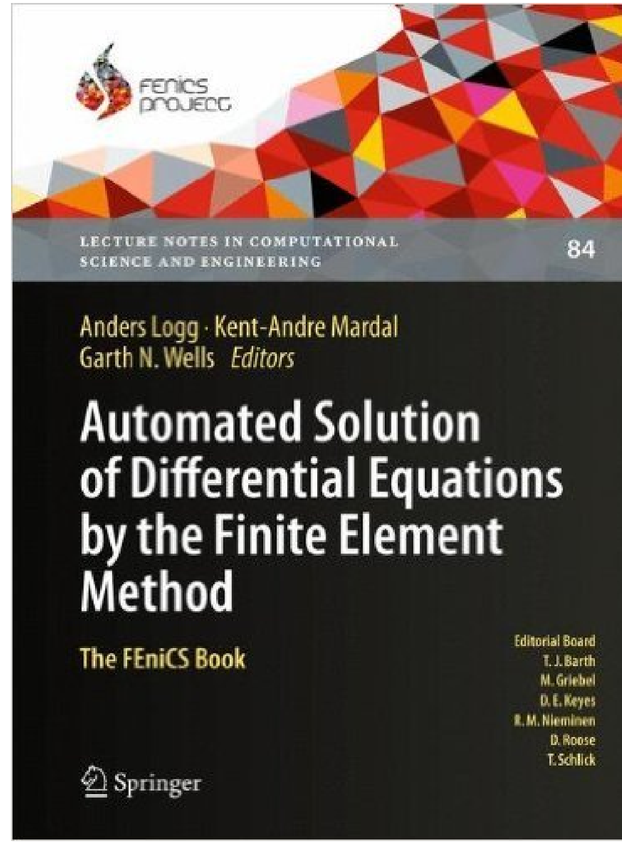
FEniCS[1]

Software

- open-source (LGPLv3)
- extensive documentation
- Python and C++ API
- can be used for HPC
- `www.fenicsproject.org`

Computing platform for solving PDEs

- Definition of weak forms
- Finite Element basis functions
- Meshing
- Solving
- ...



FEniCS book[2]

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- Solving
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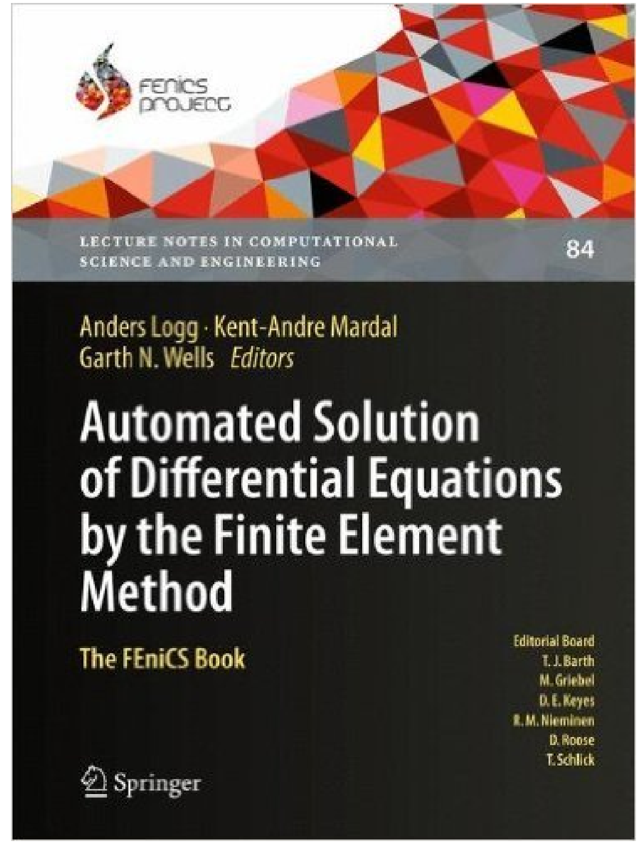
→ You can do a lot of things with FEniCS!

My goal:

Develop an official preCICE adapter for FEniCS.



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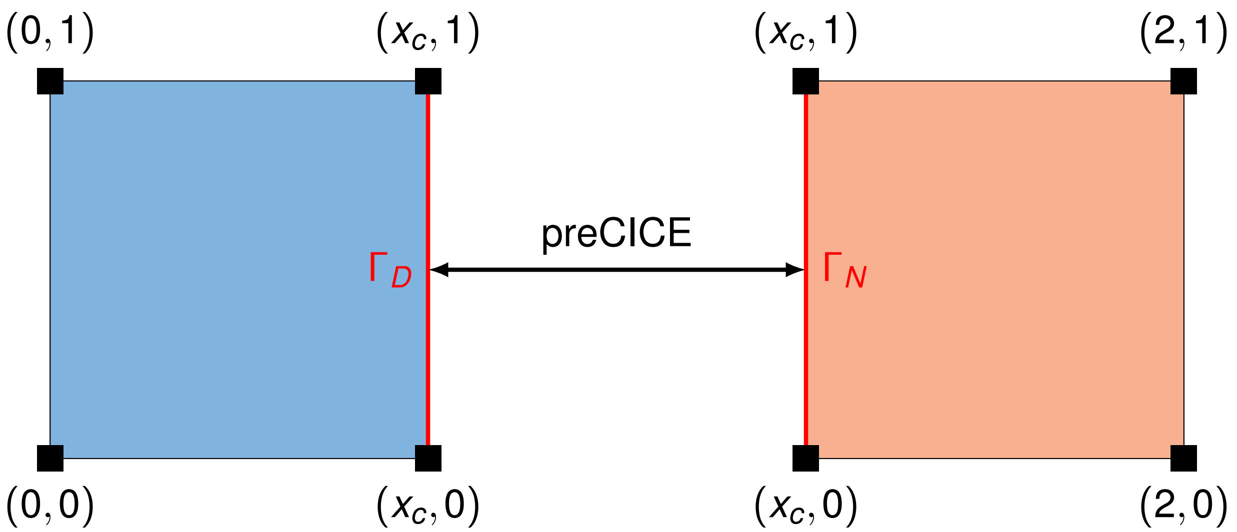
Partitioned Approach

Toy problem: Partitioned Heat Equation



Partitioned heat equation / transmission problem already discussed in literature (e.g.[1] or [2]).

[1] Monge, A. (2018). Partitioned methods for time-dependent thermal fluid-structure interaction. Lund University.

[2] Toselli, A., & Widlund, O. (2005). Domain Decomposition Methods - Algorithms and Theory (1st ed.).

Heat Equation with FEniCS

Partitioned Heat Equation

get Ω_1: $u_D = u_1(x,y)$ set Ω_2: $u_2(x,y) = u_D$

Dirichlet BC

heat equation on Ω_1

$$\frac{\partial u_1}{\partial t} = \Delta u_1 + f$$

heat equation on Ω_2

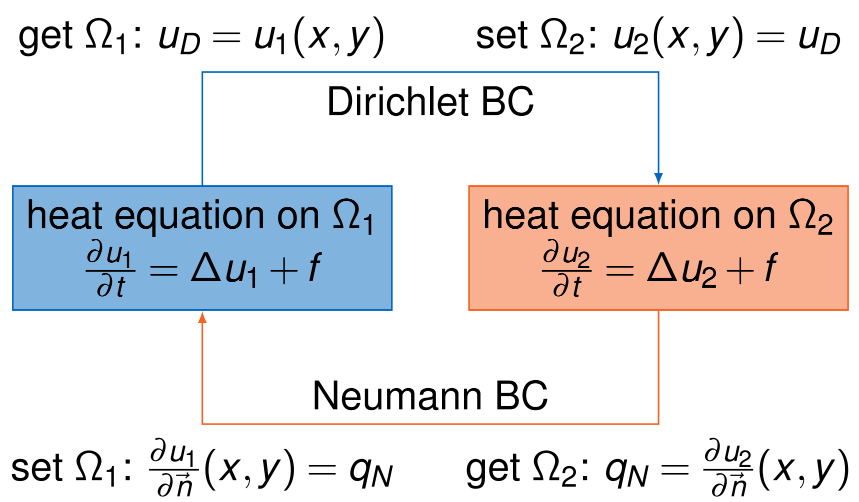
$$\frac{\partial u_2}{\partial t} = \Delta u_2 + f$$

Neumann BC

set Ω_1: $\frac{\partial u_1}{\partial \vec{n}}(x,y) = q_N$ get Ω_2: $q_N = \frac{\partial u_2}{\partial \vec{n}}(x,y)$

Heat Equation with FEniCS

Partitioned Heat Equation



FEniCS Ingredients

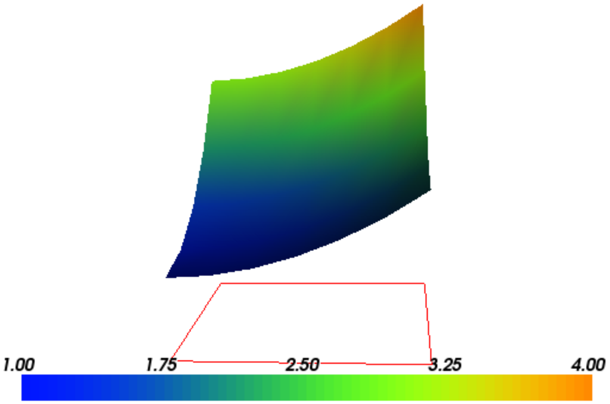
1. Solve Dirichlet Problem $\mathscr{D}(u_D)$
2. Compute heat flux $\mathscr{D}(u_D) = q_N$
3. Solve Neumann Problem $\mathscr{N}(q_N) = u_D$

Heat Equation with FEniCS

1. Solve Dirichlet Problem $\mathscr{D}(u_D)$

Heat Equation

$$\frac{\partial u}{\partial t} = \Delta u + f \text{ in } \Omega$$
$$u = u_0(t) \text{ on } \partial\Omega$$



Solution of Poisson equation. Figure from [1].

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Heat Equation with FEniCS

1. Solve Dirichlet Problem $\mathscr{D}(u_D)$

Discretization

- **implicit Euler:**

$$\frac{u^k - u^{k-1}}{dt} = \Delta u^k + f^k$$

- **trial space:**

$$u \in V_h \subset V = \left\{ v \in H^1(\Omega) : v = u_0 \text{ on } \partial\Omega \right\}$$

- **test space:**

$$v \in \hat{V}_h \subset V = \left\{ v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega \right\}$$

- **weak form:**

$$\int_\Omega (u^k v + \mathrm{d}t \nabla u^k \cdot \nabla v) \mathrm{d}x = \int_\Omega \left(u^{k-1} + \mathrm{d}t\, f^k\right) v \mathrm{d}x$$

[1] *Langtangen, H. P., & Logg, A. (2016). Solving PDEs in Python - The FEniCS Tutorial I (1st ed.).*

Heat Equation with FEniCS

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Analytical Solution

If right-hand-side $f = \beta - 2 - 2\alpha$ we get $u = 1 + x^2 + \alpha y^2 + \beta t$.

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Analytical Solution

If right-hand-side $f = \beta - 2 - 2\alpha$ we get $u = 1 + x^2 + \alpha y^2 + \beta t$.

weak form in FEniCS

```
F = u*v*dx + dt*dot(grad(u),grad(v))*dx - (u_n+dt*f)*v*dx
```

Remark: Tutorial from the FEniCS tutorial book[1]

[1] *Langtangen, H. P., & Logg, A. (2016). Solving PDEs in Python - The FEniCS Tutorial I (1st ed.).*

Heat Equation with FEniCS

2. Compute heat flux $\mathscr{D}(u_D) = q_N$

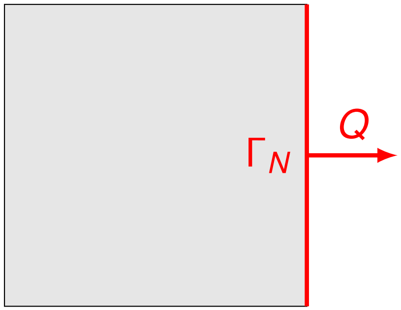
Overall Heat Flux

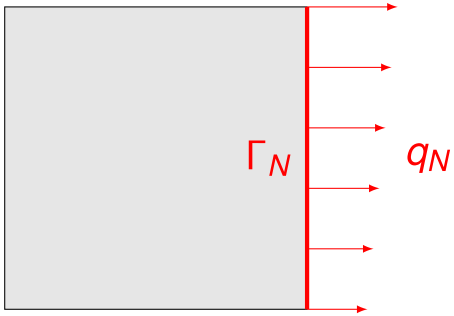
$$Q = -K \int_{\Gamma_N} \frac{\partial u}{\partial \vec{n}} \mathrm{d}s \quad (K: \text{Thermal Conductivity})$$

Elementwise Heat Flux[1]

$$\mu_i^k = \int_{\Gamma_N} \frac{\partial u^k}{\partial \vec{n}} v_i \mathrm{d}s = \int_{\Omega} u^k v_i - u^{k-1} v_i + \mathrm{d}t \nabla u^k \cdot \nabla v_i - \mathrm{d}t f^k v_i \mathrm{d}x$$

$$q_N = -K \sum_i v_i \mu_i^k$$





[1] Toselli, A., & Widlund, O. (2005). Domain Decomposition Methods - Algorithms and Theory (1st ed.). p.3 f.

Heat Equation with FEniCS

3. Solve Neumann Problem $\mathscr{N}(q_N) = u_D$

Neumann BC: Modified weak form

$$\int_\Omega (u^k v + \mathrm{d}t \nabla u^k \cdot \nabla v)\mathrm{d}x = \int_\Omega \left(u^{k-1} + \mathrm{d}t\, f^k\right) v\mathrm{d}x + \int_{\Gamma_N} q_N v\,\mathrm{d}s$$

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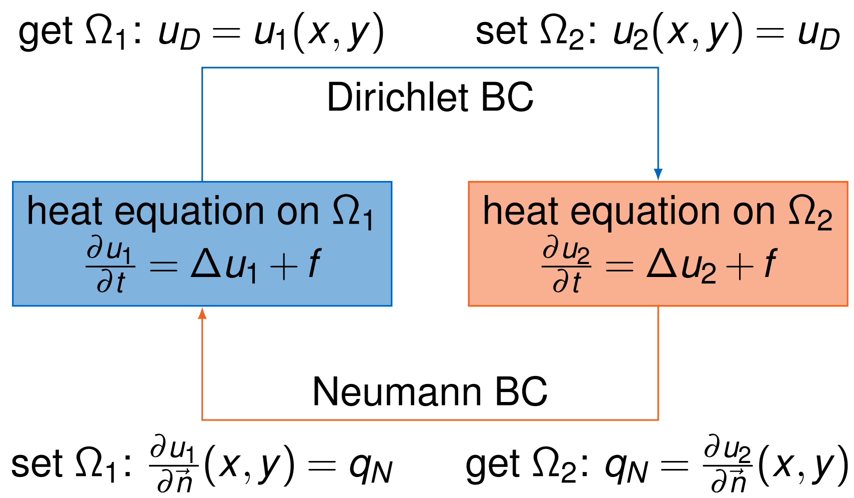
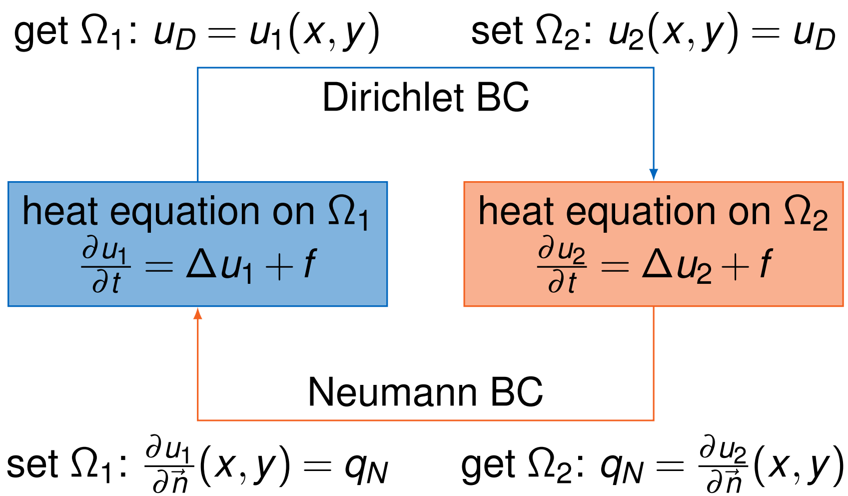
Partitioned Heat Equation



Coupling with preCICE

Partitioned Heat Equation



preCICE Ingredients

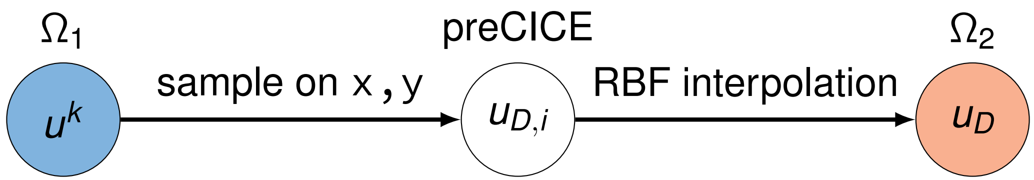
1. Read coupling data u_D, q_N to nodal data $u_{D,i}, q_{N,i}$
2. Apply coupling boundary conditions u_D, q_N
3. preCICE-FEniCS Adapter

Coupling with preCICE
1. Read Coupling Data

- Read Temperature u_D: `u_np1(x, y)`
- Read Flux q_N: `fluxes(x, y)`
- preCICE only accepts **nodal data** on the **coupling mesh**

Coupling with preCICE

2. Apply Coupling Boundary Conditions



- preCICE only returns **nodal data** on the **coupling mesh**
- use RBF interpolation to create a `CustomExpression(UserExpression)`
- Write Flux q_N as Neumann BC
- Write Temperature u_D as Dirichlet BC

Coupling with preCICE

3. preCICE-FEniCS Adapter

Example usage from the perspective of the Dirichlet solver $\mathscr{D}(u_D) = q_N$

```
from fenics import *
from fenicsadapter import Adapter
...
adapter = Adapter()
```

Coupling with preCICE

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Example usage from the perspective of the Dirichlet solver $\mathscr{D}(u_D) = q_N$

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from fenics import *
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adapter = Adapter()
adapter.configure("HeatDirichlet", "precice_config.xml",
                  "DirichletNodes", "Flux", "Temperature")
adapter.initialize(coupling_boundary, mesh, f_N_function, u_D_function)
```

Coupling with preCICE

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...
bcs = [DirichletBC(V, u_D, remaining_boundary)]
bcs.append(adapter.create_coupling_dirichlet_boundary_condition(V))
```

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while adapter.is_coupling_ongoing():
    solve(a == L, u_np1, bcs)
    fluxes = fluxes_from_temperature(F, V)
```

Coupling with preCICE

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while adapter.is_coupling_ongoing():
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    fluxes = fluxes_from_temperature(F, V)
    is_converged = adapter.advance(fluxes, dt)
    if is_converged:
        ...
```
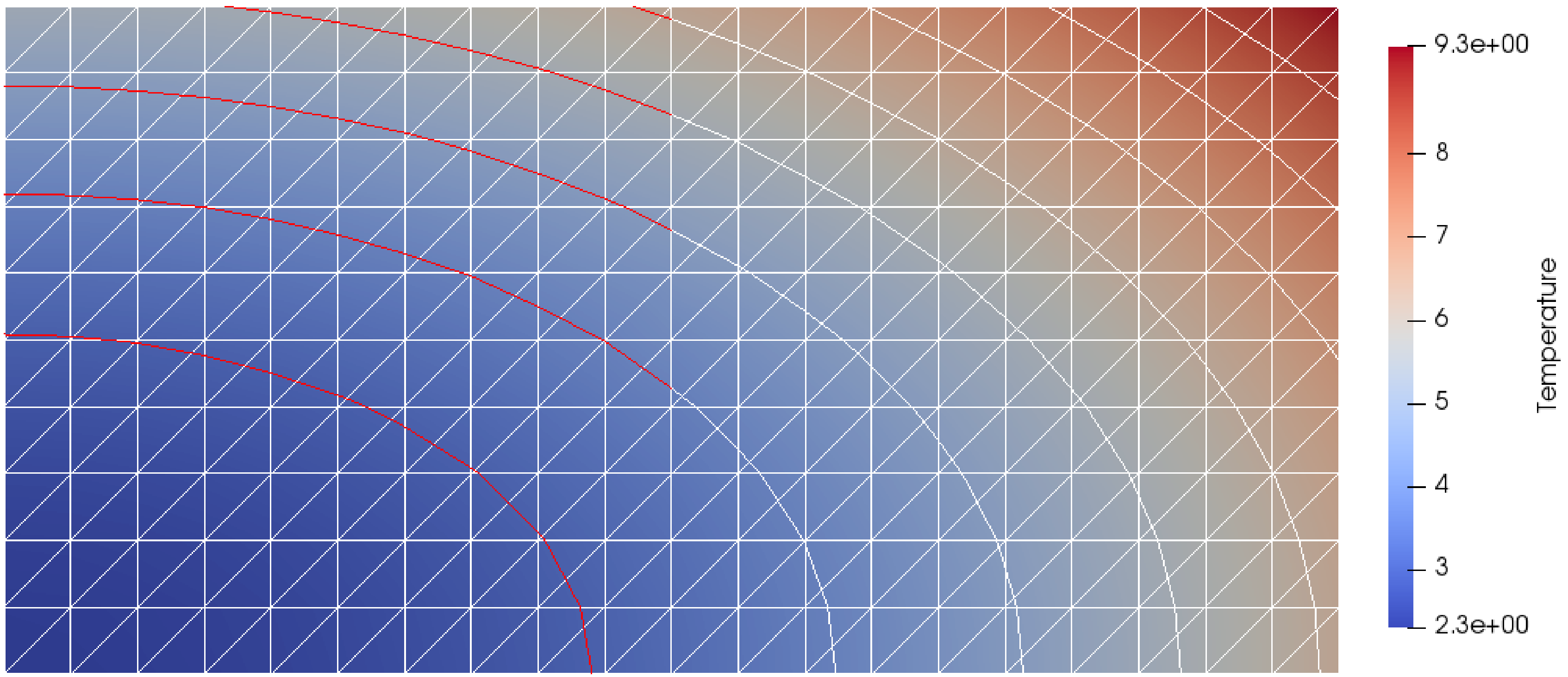

Results

Matching meshes



Comments

- simple heat equation from above
- "eyeball norm:" agreement with monolithic and analytical solution $u = 1 + x^2 + \alpha y^2 + \beta t$

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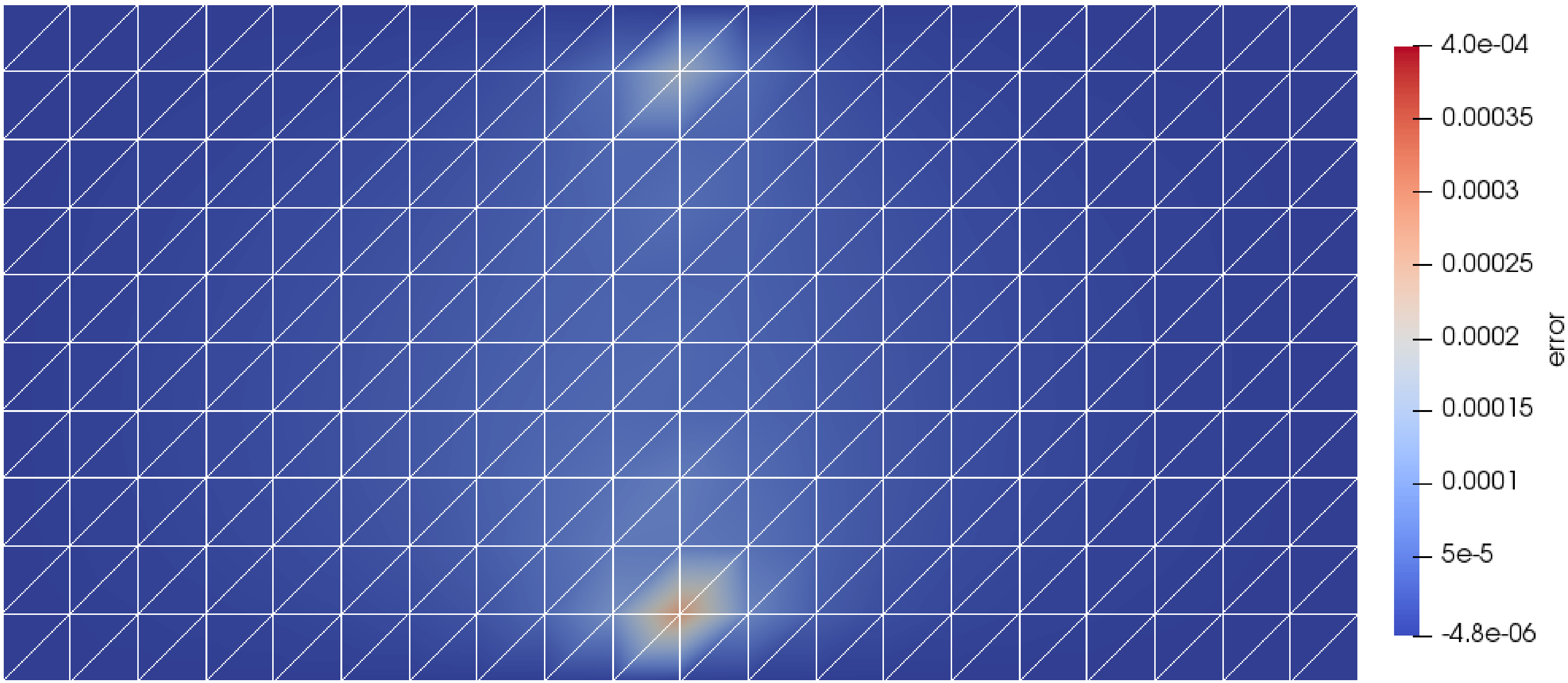
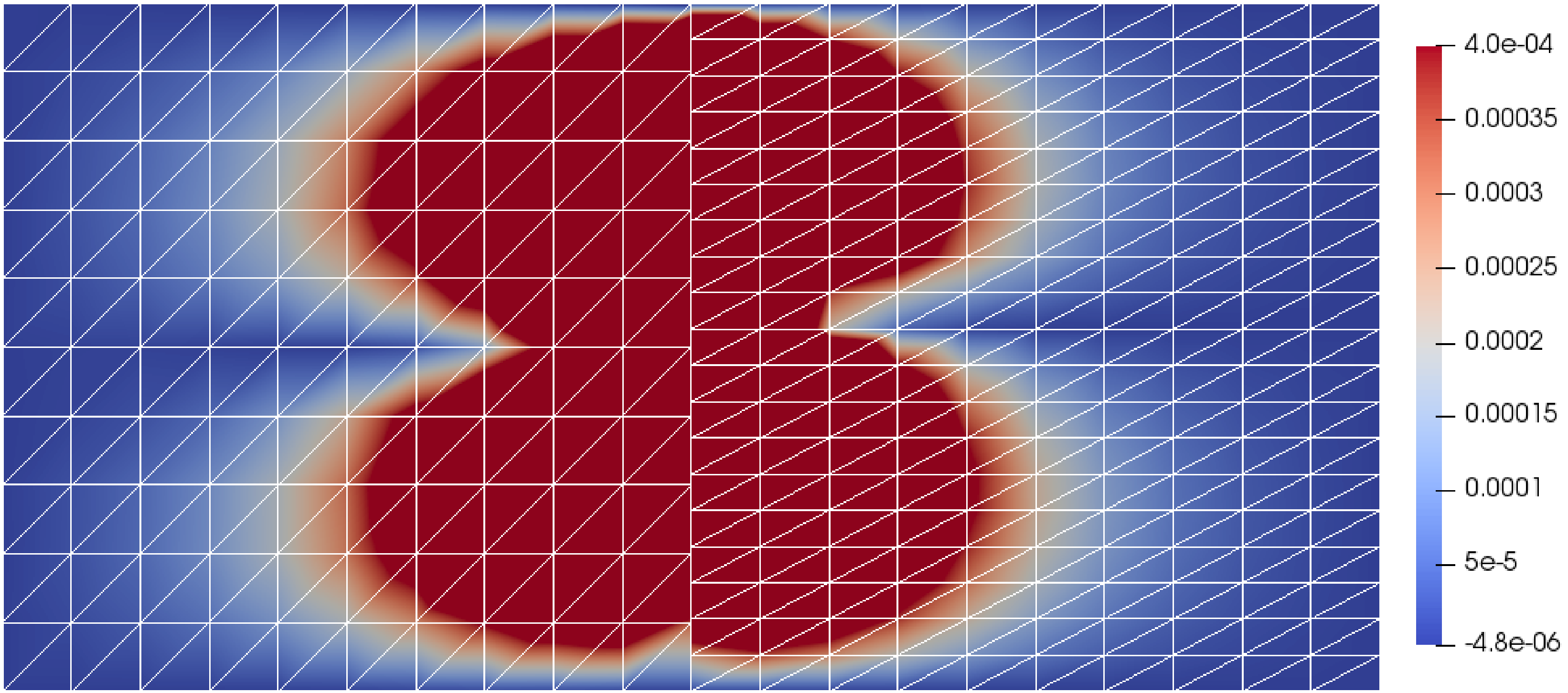


Comments

- simple heat equation from above
- "eyeball norm:" agreement with monolithic and analytical solution $u = 1 + x^2 + \alpha y^2 + \beta t$
- L^2-error on domain $< 10^{-4}$

Results

Non-matching meshes



Comments

- simple heat equation from above
- finer mesh on right domain, but larger error
- possible explanation: first order mapping destroys second order accuracy of space discretization

Summary & Outlook

Partitioned heat equation

- FEniCS is used for solving the Dirichlet and Neumann problem.
- preCICE couples two FEniCS instances to solve the coupled problem.

[1] *Langtangen, H. P., & Logg, A. (2016). Solving PDEs in Python - The FEniCS Tutorial I (1st ed.). Sec. 3.1*

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FEniCS adapter

- only minimal changes in the official FEniCS tutorial for the heat equation[1].
- FEniCS adapter for heat transport
- `github.com/precice/fenics-adapter`
- `github.com/precice/tutorials`

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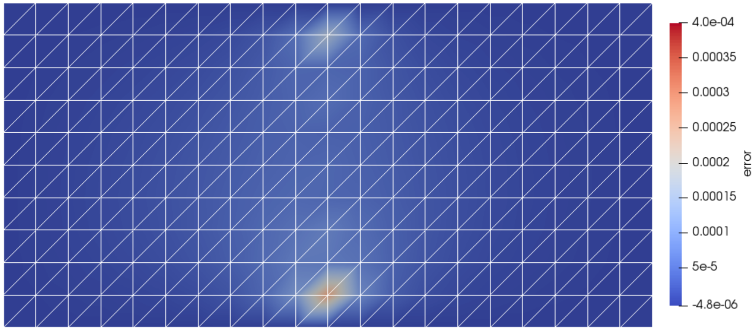
Can we live with the error close to the boundary?



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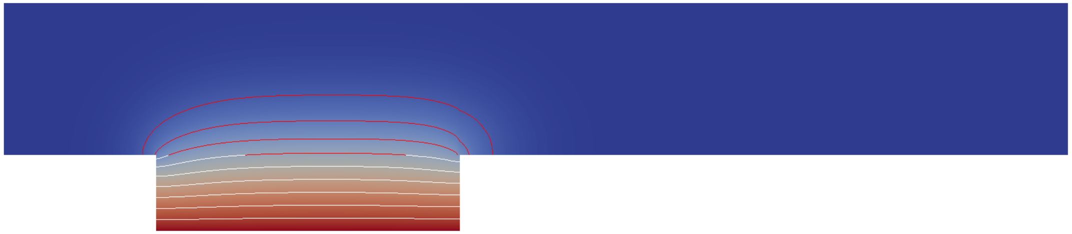
Summary & Outlook

Outlook: FEniCS + X

- first experiments with FEniCS + OpenFOAM
- more FEniCS tutorials
- FEniCS based solvers as CBC.Block, CBC.RANS and CBC.Solve[1]



Flow over heated plate. FEniCS used for solving the heat equation inside the hot plate at the bottom and OpenFOAM used for simulation of the channel flow.

[1] *Logg, A., Mardal, K. A., & Wells, G. N. (2012). Automated solution of differential equations by the finite element method. Lecture Notes in Computational Science and Engineering.*

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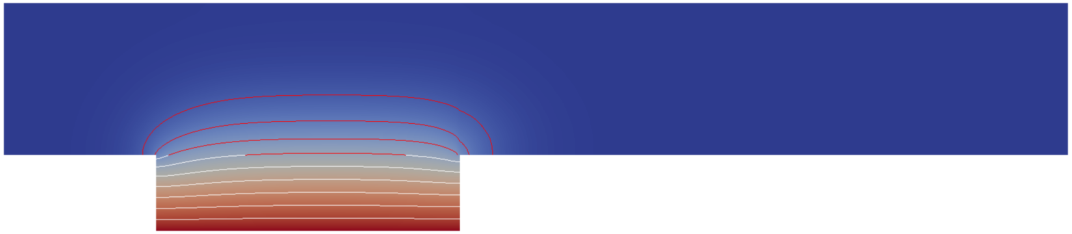

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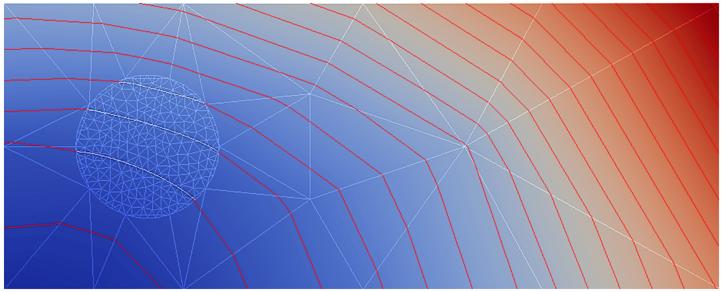
Non-matching Meshes



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Thank You!

Website: `precice.org`
Source/Wiki: `github.com/precice`
Mailing list: `precice.org/resources`
My e-mail: `rueth@in.tum.de`

Homework:

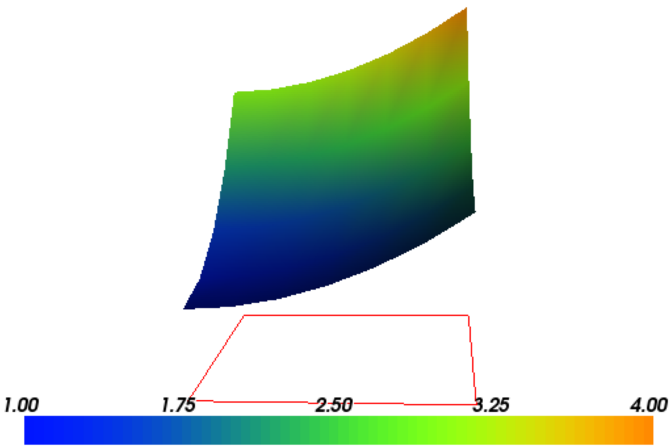
- Follow a tutorial
- Join our mailing list
- Star on GitHub
- Send us feedback
- Ask me for stickers

Dirichlet Problem with FEniCS

Heat Equation

$$\frac{\partial u}{\partial t} = \Delta u + f \text{ in } \Omega$$
$$u = u_0(t) \text{ on } \partial\Omega$$

Analytical Solution, if $f = \beta - 2 - 2\alpha$ we get $u = 1 + x^2 + \alpha y^2 + \beta t$.



Solution of Poisson equation. Figure from [1].

Discretization

- **implicit Euler:**

$$\frac{u^k - u^{k-1}}{dt} = \Delta u^k + f^k$$

- **trial space:**

$$u \in V_h \subset V = \left\{ v \in H^1(\Omega) : v = u_0 \text{ on } \partial\Omega \right\}$$

- **test space:**

$$v \in \hat{V}_h \subset V = \left\{ v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega \right\}$$

- **weak form:**

$$\int_\Omega (u^k v + \mathrm{d}t \nabla u^k \cdot \nabla v) \mathrm{d}x = \int_\Omega \left(u^{k-1} + \mathrm{d}t\, f^k \right) v \mathrm{d}x$$

Remark: Tutorial from the FEniCS book[1]

[1] *Langtangen, H. P., & Logg, A. (2016). Solving PDEs in Python - The FEniCS Tutorial I (1st ed.).*

Dirichlet Problem with FEniCS

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Geometry: $\Omega, \partial\Omega, \Gamma_D, \Gamma_N$

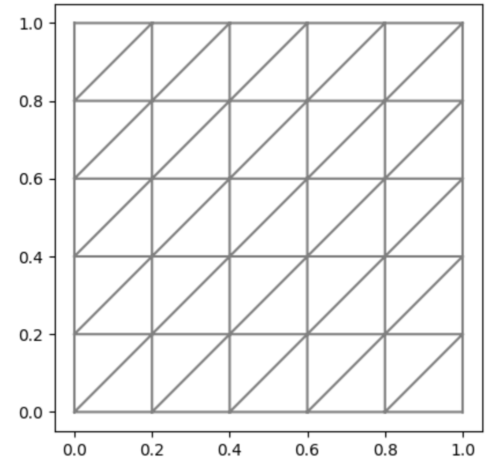
```
class RightBoundary(SubDomain):
    def inside(self, x, on_boundary):
        tol = 1E-14
        if on_boundary
           and near(x[0], x_r, tol):
            return True
        else:
            return False

class Boundary(SubDomain):
    def inside(self, x, on_boundary):
        if on_boundary:
            return True
        else:
            return False

p0 = Point(0, 0)
p1 = Point(1, 1)
```

Mesh: Ω_h

```
nx = 5
ny = 5
mesh = RectangleMesh(p0, p1,
                     nx, ny)
```



Mesh created with FEniCS

Dirichlet Problem with FEniCS

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Function Space: $V_h \subset V = \left\{ v \in H^1(\Omega) \right\}$

```
V = FunctionSpace(mesh, 'P', 1)
```

Expressions: $u = 1 + x^2 + \alpha y^2 + \beta t$ and $f = \beta - 2 - 2\alpha$

```
u_D = Expression('1 + x[0]*x[0] + alpha*x[1]*x[1] + beta*t', ..., t=0)
f = Constant(beta - 2 - 2 * alpha)
```

Boundary Conditions: $u \in V_h \subset V = \left\{ v \in H^1(\Omega) : v = u_D \text{ on } \partial\Omega \right\}$ and $v \in \hat{V}_h \subset V = \left\{ v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega \right\}$

```
bc = DirichletBC(V, u_D, Boundary)
u = TrialFunction(V)
v = TestFunction(V)
```

Initial Condition: $u^0 = u(t = 0)$

```
u_n = interpolate(u_D, V)
```

Dirichlet Problem with FEniCS

Variational Problem: $\int_\Omega (u^k v + dt \nabla u^k \cdot \nabla v) dx = \int_\Omega \left(u^{k-1} + dt f^k\right) v dx$

```
F = u * v * dx + dt * dot(grad(u), grad(v)) * dx - (u_n + dt * f) * v *
    dx
a, L = lhs(F), rhs(F)
```

Time-stepping and simulation loop: $\frac{u^k - u^{k-1}}{dt} = \Delta u^k + f^k$

```
u_np1 = Function(V)
t = 0
T = 1
dt = .1
u_D.t = t + dt

while t < T:
    solve(a == L, u_np1, bc)
    t += dt
    u_D.t = t + dt
    u_n.assign(u_np1)
```