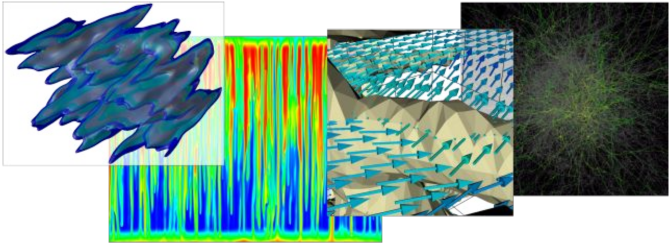
DUNE PDELab Tutorial 09

Using Code Generation to Create Local Operators



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Introduction

We will look at a quick example to get some idea how this looks like.

Hello World: Poisson Problem

- Strong formulation:

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ u &= g && \text{on } \partial\Omega, \end{aligned}$$

- Discrete weak formulation: Find $u_h \in U_h$ with

$$r_h^{Poisson}(u_h, v_h) = \int_\Omega \nabla u_h \cdot \nabla v_h \, dx - \int_\Omega f \, v_h \, dx = 0 \qquad \forall v_h \in V_h$$

- Parameter functions:

$$\begin{aligned} f(x) &= -2d \\ g(x) &= \|x\|_2^2 \end{aligned}$$

UFL file for Poisson Problem

Discrete weak formulation: Find $u_h \in U_h$ with

$$r_h^{Poisson}(u_h, v_h) = \int_\Omega \nabla u_h \cdot \nabla v_h \, dx - \int_\Omega f \, v_h \, dx = 0 \qquad \forall v_h \in V_h$$

```
cell = triangle
V = FiniteElement("CG", cell, 1)
u = TrialFunction(V)
v = TestFunction(V)

dim = 2
x = SpatialCoordinate(cell)
g = x[0]*x[0]+x[1]*x[1]
f = -2*dim

r = inner(grad(u), grad(v)) * dx \
  - f*v * dx

# dune-codegen specific
exact_solution = g
interpolate_expression = g
is_dirichlet = 1
```

Introduction

Introduction

- dune-codegen[1] is a seperate module
- This tutorial gives a short introduction to using dune-codegen
- dune-codegen uses code generation to solve PDEs. This is done by describing the PDE in a domain-specific language (DSL) and generating C++ code for the local integration kernels
- We use UFL[2] as DSL
- The generated code can be used in dune-pdelab
- This makes it easier to use PDELab for your application

[1] https://gitlab.dune-project.org/extensions/dune-codegen
[2] https://bitbucket.org/fenics-project/ufl

Goals of this Talk

Goals of this talk

- Explain how to write down PDEs in UFL
- Show how `dune-codegen` modifies/extends UFL
- Show how it is integrated into the build system

Before this we will

- Give a short overview over the workflow
- Talk about differences to other code generation approaches

Resources

This tutorial is partially based on

- “Code Generation for High Performance PDE Solvers on Modern Architectures” by Dominic Kempf
- “Unified Form Language: A domain-specific language for weak formulations of partial differential equations” M. S. Alnaes, A. Logg, K. B. Ølgaard, M. E. Rognes and G. N. Wells
- UFL documentation `https://fenics.readthedocs.io/projects/ufl/en/latest/index.html`

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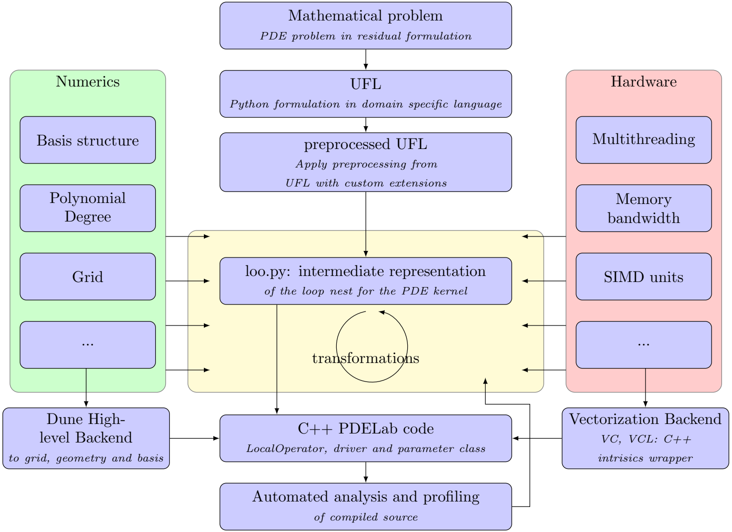
The Big Picture

- Research goals of `dune-codegen`:
  - Generate high performance code
  - Performance optimizations on intermediate representation
- Difference to other code generation approaches:
  - Only generate local integration kernels and use framework around it
  - The workflow is CMake and C++ driven and not controlled by Python
  - Main focus on generating high performance code

Typical Workflow

- Have a dune module that depends on `dune-codegen`
- Write a UFL file describing the PDE
- Add a target in CMake (see build system part)
- Go to the build directory and type make
- dune-codegen will generate the localoperator including the jacobian methods
- After generating the localoperator CMake will compile your executable

Form Compiler Approach



Contents

UFL: Poisson

Discrete weak formulation: Find $u_h \in U_h$ with

$$r_h^{Poisson}(u_h, v_h) = \int_\Omega \nabla u_h \cdot \nabla v_h \, dx - \int_\Omega f \, v_h \, dx = 0 \qquad \forall v_h \in V_h$$

```
cell = triangle
V = FiniteElement("CG", cell, 1)
u = TrialFunction(V)
v = TestFunction(V)

dim = 2
x = SpatialCoordinate(cell)
g = x[0]*x[0]+x[1]*x[1]
f = -2*dim

r = inner(grad(u), grad(v)) * dx \
  - f*v * dx

# dune-codegen specific
exact_solution = g
interpolate_expression = g
is_dirichlet = 1
```

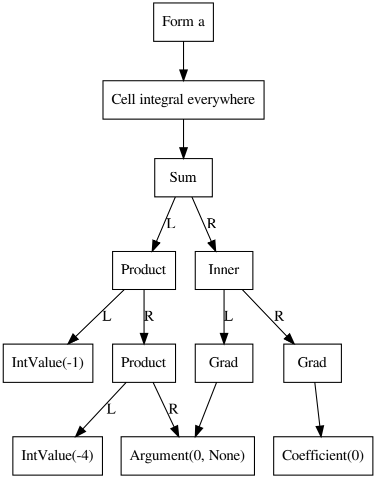
UFL: About

- Domain specific language for describing weak formulations of PDE discretizations
- Notation stays close to mathematical formulation
- Embedded in Python
- Only desribes cell/facet local computations. There is no notion of a grid or a description of an element loop
- The form is described by an abstract syntax trees (AST)
- UFL can apply transformation on the AST e.g.:
  - Calculation of the Jacobian of the residual
  - Geometry lowering

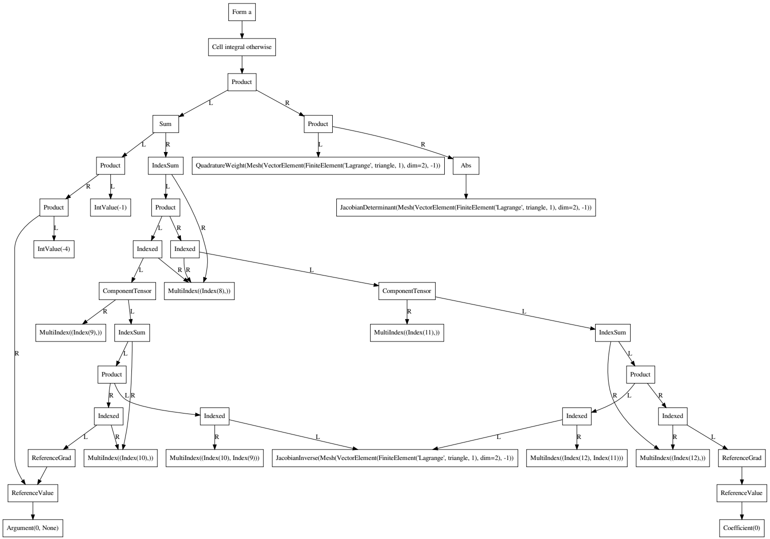
UFL: AST

The weak formulation was:

$$r_h^{Poisson}(u, v) = (\nabla u, \nabla v)_{0,\Omega} - (-2\,dim, v)_{0,\Omega}$$



UFL: AST - Preprocessed



UFL: File

Next step: Break down content of UFL file

```
cell = triangle
V = FiniteElement("CG", cell, 1)
u = TrialFunction(V)
v = TestFunction(V)

dim = 2
x = SpatialCoordinate(cell)
g = x[0]*x[0]+x[1]*x[1]
f = -2*dim

r = inner(grad(u), grad(v)) * dx \
  - f*v * dx

# dune-codegen specific
exact_solution = g
interpolate_expression = g
is_dirichlet = 1
```

UFL: FiniteElement

```
cell = triangle
V = FiniteElement("CG", cell, 1)
```

- family: String representing a finite element family
  - 'CG' Continuous Lagrange finite element
  - 'DG' Discontinuous Galerkin Lagrange finite element
- Possible Cells:

Dimension	Simplex Cell	Cube Cell
0	vertex	vertex
1	interval	interval
2	triangle	quadrilateral
3	tetrahedron	hexahedron

- Instead you can also write Cell('triangle')
- degree: Polynomial degree

UFL: TrialFunction and TestFunction

```
u = TrialFunction(V)
v = TestFunction(V)
```

- TrialFunction and TestFunction represent finite element functions.
- Take FiniteElement as argument
- Note: The mathematical residual will always be linear in the test function but might be nonlinear in the ansatz function

UFL: Defining Expressions

```
dim = 2
x = SpatialCoordinate(cell)
g = x[0]*x[0]+x[1]*x[1]
f = -2*dim

r = inner(grad(u), grad(v)) * dx \
  - f*v * dx
```

- `SpatialCoordinate`: Global coordinate
- `grad(u)`: Gradient of u
- `inner(A,B)`: Inner product

$$A : B = \sum_{i_0} \cdots \sum_{i_{n-1}} A_{i_0 \cdots i_{n-1}} B_{i_0 \cdots i_{n-1}}$$

- `dx`: Multiplication with `dx` indicates a volume integral

UFL: Form

- Integrals (and sums of integrals) are called forms
- UFL expresses forms

$$\begin{aligned} a : W_1 \times \cdots \times W_m \times V_1 \times \cdots \times V_n &\to \mathbb{R} \\ (w_1, \ldots, w_m, v_1, \ldots, v_n) &\mapsto a(w_1, \ldots, w_m; v_1, \ldots, v_n) \end{aligned}$$

- Linear in the arguments $v_1, \ldots, v_n$
- Possibly nonlinear in coefficient functions $w_1, \ldots, w_m$
- PDELab uses a residual formulation: Find $u \in U$ with

$$r(u, v) = 0 \qquad \forall v \in V$$

- r is linear in v but might be nonlinear in u

UFL: dune-codegen Specific

```
# dune-codegen specific
exact_solution = g
interpolate_expression = g
is_dirichlet = 1
```

- Main goal of dune-codegen is to generate the local integration kernel
- For testing and solving simple problem an automated driver can be generated. For the correct handling of the boundary condition we need to add some information to the UFL file
- `exact_solution`: Can be set for writing tests if solution is known
- `is_dirichlet`: Expression that may depend on x and returns 1 if this is a dirichlet boundary condition. This is used only for driver generation.
- `interpolate_expression`: This is used as Dirichlet boundary value

UFL: Poisson

One last time the complete UFL file:

```
cell = triangle
V = FiniteElement("CG", cell, 1)
u = TrialFunction(V)
v = TestFunction(V)

dim = 2
x = SpatialCoordinate(cell)
g = x[0]*x[0]+x[1]*x[1]
f = -2*dim

r = inner(grad(u), grad(v)) * dx \
  - f*v * dx

# dune-codegen specific
exact_solution = g
interpolate_expression = g
is_dirichlet = 1
```

Contents

UFL: Towards More Complex Forms

In the following we show some important features of UFL. This is by no means complete, see the official documentation for further details `https://fenics.readthedocs.io/projects/ufl/en/latest/index.html`.

UFL: Math Expressions

- Math functions, e.g. `*`, `/`, `+`, `-`, `abs`, `exp`, `ln`, `sqrt`, trigonometric functions, ...
- Comparison operator: `eq`, `ne`, `le`, `ge`, `lt` and `gt`
- Conditionals:

$$\texttt{conditional(cond, A, B)} = \begin{cases} \texttt{A} & \texttt{cond is True} \\ \texttt{B} & \texttt{cond is False} \end{cases}$$

- Vector-, matrix- and tensor-valued objects can be created through `as_vector`, `as_matrix` and `as_tensor`

```
a = as_matrix([[1.0, 2.0],[3.0, 4.0]])
```

- See the official documentation for tensor algebra operations

UFL: Geometric Quantities

- `SpatialCoordinate(cell)`: Global coordinate
- `FacetNormal(cell)`: Unit outer normal vector
- `CellVolume(cell)` and `FacetArea(cell)`

UFL: Integral Measures

- Multiplication with a measure describes an integral object over a local cell or facet
- `dx`: Integral over cell
- `ds`: Integral over boundary facet
- `dS`: Integral over interior facet
- Measures can be restricted to a subdomain. See the example about mixed Dirichlet and Neumann conditions on the next slides

Example: Mixed Boundary Conditions

Strong formulation:

$$
\begin{aligned}
-\Delta u + q(u) &= f && \text{in } \Omega, \\
u &= g && \text{on } \Gamma_D \subset \partial\Omega, \\
-\nabla u \cdot \nu &= j && \text{on } \Gamma_N \subset \partial\Omega
\end{aligned}
$$

Weak discrete formulation: Find $u_h \in U_h$ with

$$
\begin{aligned}
r_h^{NLP}(u_h, v_h) = \int_\Omega \nabla u_h \cdot \nabla v_h \, dx + \int_\Omega q(u) \, v \, dx \\
- \int_\Omega f \, v_h \, dx + \int_{\Gamma_N} j \, v \, ds = 0 \qquad \forall v_h \in V_h
\end{aligned}
$$

Parameter functions:

$$
\begin{aligned}
f(x) &= -2d \\
g(x) &= \|x\|_2^2 \\
j(x) &= -\begin{pmatrix} 2x_0 \\ 2x_1 \end{pmatrix} \cdot \nu
\end{aligned}
$$

Example: Mixed Boundary Conditions

```
V = FiniteElement("CG", triangle, 1)
u = TrialFunction(V)
v = TestFunction(V)

x = SpatialCoordinate(triangle)
dim = 2
eta = 2
g = x[0]*x[0]+x[1]*x[1]
f = -2*dim+eta*g*g

def q(u):
    return eta*u*u

# Decide where to apply which boundary
# 0: Neumann
# 1: Dirichlet
bctype = conditional(Or(x[0]<1e-8, x[0]>1.-1e-8), 0, 1)
sgn = conditional(x[0] > 0.5, 1., -1.)
j = -2.*sgn*x[0]

# Define the boundary measure that knows where we are...
ds = ds(subdomain_data=bctype)

r = inner(grad(u), grad(v))*dx + q(u)*v*dx - f*v*dx + j*v*ds(0)

exact_solution = g
is_dirichlet = bctype
interpolate_expression = g
```

UFL: DG Operators

UFL provides operators for implementation of Discontinuous Galerkin (DG) methods. These methods are discontinuous at interior facets. This means you have two values there: One for the 'inside' cell and one for the 'outside' cell.

- `avg(u)`: Average between those values $\frac{1}{2}(u|_{T^+} + u|_{T^-})$
- `jump(u)`: Difference between the values $u|_{T^+} - u|_{T^-}$
- Restriction: Expression can be restricted to the inside or the outside cell by typing `u('+')` or `u('-')`
- **Note:** UFL denotes the inside cell with "+" and the outside cell with "-" so we stick to this convention for dune-codegen. In the literature this is usually done the other way round.
- We will see an example on the exercise sheet.

UFL: FiniteElement

VectorElement

V= VectorElement(family, cell , degree [, size])

- Combination of a basic element for a vector field
- `family`, `cell`, `degree` like `FiniteElement` above
- `size`: Optional, default equal to dimension

TensorElement

V = TensorElement(family, cell , degree [, shape, symmetry])

- Like `VectorElement` but for `shape` given as tuple
- Symmetry can be expressed as Python dictionary `symmetry={(0,1): (1,0)}`

MixedElement

V = MixedElement(element1, element2 [,...])

- Arbitrary combination of finite elements
- Can also be created like this `V = element1*element2`

UFL: Trialfunctions and Testfunctions

- You can get the test- and trialfunctions of these spaces using the `split` command

```
FE_V = VectorElement('CG', triangle, 2)
FE_P = FiniteElement('CG', triangle, 1)
TH = FE_V * FE_P
u, p = split(TrialFunction(TH))
v, q = split(TestFunction(TH))
```

- There is also an abbreviation (don't miss the additional s)

```
u, p = TrialFunctions(TH)
v, q = TestFunctions(TH)
```

Example: Wave Equation as First Order System

Strong formulation as first order system:

$$
\begin{aligned}
\partial_t u_1 - c^2 \Delta u_0 &= 0 && \text{in } \Omega \times \Sigma, \\
\partial_t u_0 - u_1 &= 0 && \text{in } \Omega \times \Sigma, \\
u_0 &= 0 && \text{on } \partial\Omega, \\
u_1 &= 0 && \text{on } \partial\Omega, \\
u_0 &= q && \text{at } t = 0, \\
u_1 &= w && \text{at } t = 0.
\end{aligned}
$$

Weak discrete formulation: Find $(u_0(t), u_1(t)) \in U_0 \times U_1$ s.t.

$$
\begin{aligned}
d_t(u_1, v_0)_{0,\Omega} + c^2(\nabla u_0, \nabla v_0)_{0,\Omega} &= 0 \quad \forall v_0 \in U_0 \\
d_t(u_0, v_1)_{0,\Omega} - (u_1, v_1)_{0,\Omega} &= 0 \quad \forall v_1 \in U_1
\end{aligned}
$$

Parameters: Speed of sound $c = 1$

Example: Wave Equation as First Order System

$$
\begin{aligned}
d_t(u_1, v_0)_{0,\Omega} + c^2(\nabla u_0, \nabla v_0)_{0,\Omega} &= 0 \quad \forall v_0 \in U_0 \\
d_t(u_0, v_1)_{0,\Omega} - (u_1, v_1)_{0,\Omega} &= 0 \quad \forall v_1 \in U_1
\end{aligned}
$$

```
cell = quadrilateral

V = VectorElement("CG", cell, 1)
u0, u1 = TrialFunctions(V)
v0, v1 = TestFunctions(V)

c = 1.0

mass = inner(u1, v0) * dx \
     + inner(u0, v1) * dx

r = c**2 * inner(grad(u0), grad(v0)) * dx \
  - inner(u1, v1) * dx
```

UFL: Derivatives

- `grad(u)`: Gradient of u
- `div(u)`: Divergence of u
- `curl(u)`: Curl of u (only for finite element functions with three components)
- `u.dx(d)`: D'th partial derivative $\frac{\partial u}{\partial x_d}$
- UFL can also compute derivatives of forms or expressions wrt to `Variables` or `Coefficients` (Note: In `dune-codegen` the `TrialFunction` is a `Coefficient`)

```
# Define arbitrary expression
u = Coefficient(element)
w = sin(u**2)

# Annotate expression w as a variable that can be used by 'diff'
w = variable(w)

# Derivative of expression F
F = w**2
dF_w = diff(F, w)
dF_u = diff(F, u)
```

UFL: dune-codegen Specific

- As mentioned before dune-codegen uses the residual formulation. The provided residual form may be nonlinear in the trial function.[3]
- Your UFL file may contain multiple forms. dune-codegen will generate local operators for all forms listed in the ini file, eg

```
[formcompiler]
operators = mass, poisson
```

- See the build system part of this tutorial for more options!

[3] In our case the trialfunction is a Coefficient and not an Argument.

UFL: dune-codegen Specific

- For testing automated drivers can be generated. We use the following convention for instationary problems: If there are exactly two forms and one is called mass we assume that the problem is instationary and generate a suitable driver.[4]
- Instationary problems can have time dependent parameters but UFL has no notion of time. In dune-codegen you can get a variable representing the time by

```
t = get_time(cell)
```

[4] Keep in mind that dune-codegen was developed to generate local operator. The driver generation was mainly done for testing.

Example: Heatequation

```
cell = quadrilateral

x = SpatialCoordinate(cell)
time = get_time(cell)

g = cos(2*pi*time)*cos(pi*x[0])**2*cos(pi*x[1])**2

V = FiniteElement("CG", cell, 1)
u = TrialFunction(V)
v = TestFunction(V)

mass = (u*v)*dx
poisson = inner(grad(u), grad(v))*dx

interpolate_expression = g
is_dirichlet = 1
```

Contents

CMake: dune_add_generated_executable

- We need to generate C++ code and compile it
- Add a code generation target to your CMakeLists.txt

```
dune_add_generated_executable(
    UFLFILE uflfile
    INIFILE inifile
    TARGET target
    [SOURCE source]
)
```

- UFLFILE: UFL file describing the PDE
- INIFILE: Ini file with code generation option under [formcompiler] section
- TARGET: Name of the executable
- SOURCE: C++ file used for building the target. This is optional, if omitted a minimal driver willl be generated

CMake: dune_add_generated_executable

- Automated driver generation was mainly developed for automated software tests
- For complicated applications handwritten drivers will be necessary. This requires control over the file- and classname of the generated local operator.
- Can be done in the ini file

```
[formcompiler]
operators = r
...

[formcompiler.r]
filename = r_operator.hh
classname = ROperator
```

Ini File: [formcompiler] Options

- Put into the [formcompiler] section
- operators: Comma separated list of form names for which we want to generate operators [default r]. Example:

```
[formcompiler]
operators = mass, poisson
```

- explicit_time_stepping: Use explicit time stepping (in instationary case) [0/1, default 0]. Example:

Ini File: Form Options under [formcompiler.formname]

- Options for a form called `r` need to be put into the `[formcompiler.r]` section
- `filename`: Name of the generated local operator file `[str, optional]`
- `classname`: Name of the local operator class `[str, optional]`
- `numerical_jacobian`: Use numerical differentiation for assembling the Jacobian of the residual `[0/1, default 0]`
- `quadrature_order`: Order of quadrature `[int>0,],optional, guessed by UFL if omitted)`
- `geometry_mixins`: Information about grid properties that can lead to simplified gemometry evaluations `[generic/axiparallel/equidistant]`

Ini File: Options for Generated Driver

Grid generation

- Grid generation options are at the top under no section
- Quadrilateral grid

```
cells = 32 32
extension = 1. 1.
```

- Simplex grid

```
lowerleft = 0.0 0.0
upperright = 1.0 1.0
elements = 32 32
elementType = simplical
```

- Gmsh grid

```
gmshFile = cylinder2dmesh1.msh
```

Ini File: Options for Generated Driver

Name of vtk output

- Under section [wrapper.vtkcompare]
- name: Basename (without ending) of vtk output

Parameters for Instationary problems

- Need to be put into the [instat] section
- T: End of time intervall
- dt: Time step size
- output_every_nth: Write visualization output for every nth time step

CMake: Example Heatequation

```
cell = quadrilateral

x = SpatialCoordinate(cell)
time = get_time(cell)

V = FiniteElement("CG", cell, 1)
u = TrialFunction(V)
v = TestFunction(V)

mass = (u*v)*dx
poisson = inner(grad(u), grad(v))*dx

# This example uses a hand written driver so these ar not needed!
# g = cos(2*pi*time)*cos(pi*x[0])**2*cos(pi*x[1])**2
# interpolate_expression = g
# is_dirichlet = 1
```

CMakeLists.txt

```
dune_add_generated_executable(TARGET heatequation
                              UFLFILE heatequation.ufl
                              INIFILE heatequation.ini
                              SOURCE heatequation_driver.cc
                              )

dune_symlink_to_source_files(FILES heatequation.ini)
```

CMake: Example Heatequation

heatequation.ini

```
cells = 32 32
extension = 1. 1.

[wrapper.vtkcompare]
name = heatequation

[instat]
T = 1
dt = 0.01
output_every_nth = 5

[formcompiler]
operators = mass, poisson
explicit_time_stepping = 0

[formcompiler.mass]
filename = heatequation_mass_operator.hh
classname = MassOperator
geometry_mixins = equidistant

[formcompiler.poisson]
filename = heatequation_poisson_operator.hh
classname = PoissonOperator
geometry_mixins = equidistant
```

Examples

In the folder `tutorial09/src` you can find several examples:

- Poisson equation from tutorial00
- Nonlinear Poisson equation with mixed boundary from tutorial01
- Heat equation from tutorial03
- Wave equation from tutorial04

In the exercises you will additionally find examples for:

- Navier Stokes equation modeling the flow around a cylinder from tutorial08
- Discontinuous Galerkin discretization of the Poisson equation