Programming large systems of PDEs in Python via cbc.pdesys

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Specifying large systems of PDEs with ease

This article describes the cbc.pdesys Python package, built on top of FEniCS, for specifying and solving systems of nonlinear PDEs with very compact and flexible code.

About solving large systems of nonlinear PDEs

Computational Fluid Dynamics (CFD) presents many tough challenges for a scientific computing software. The Navier-Stokes equations that are used to model Newtonian fluid flows are represented by a nonlinear system of PDEs, where velocity is non trivially coupled with pressure – and that is just the beginning. The fluid may also interact with solid objects, flames, particles or simply another fluid with a different density. Most applications we investigate today are built by adding more and more PDE systems on top of the basic fluid flow model. For example, to study combustion we need to couple the Navier-Stokes equations with a turbulence model and several (often more than 10) nonlinear scalar transport equations, one for each of the reacting species. Combustion is hot, so we have to incorporate the energy equation in the model system of PDEs as well. Each of the three components (Navier-Stokes, turbulence model and combustion) of the complete model problem is represented by its own system of PDEs.

In fact, the needs of CFD is simply a very flexible software environment for systems of nonlinear PDEs. To meet these needs, we created the completely general `cbc.pdesys` Python package on top of FEniCS. The purpose of the package is to offer the computational scientist an efficient way of

- specifying possibly large, complicated systems of PDEs,

- dividing each system of PDEs into subsystems that are solved either fully coupled or segregated,
- linearizing nonlinear PDEs in a flexible way (Picard or Newton strategies),

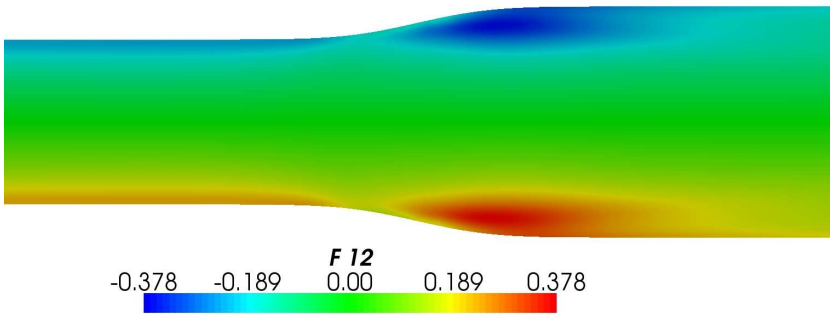
The package targets any system of PDEs, but the applications so far have been restricted to CFD. The stream-functions above illustrating flow past a dolphin is computed in the tutorial given below.

Proof of concept – The elliptic relaxation model

Reynolds Averaged Navier-Stokes (RANS) models are widely used in industry for modeling statistical properties of turbulent flows. One of the most advanced RANS models around is the elliptic relaxation model. This model consists of the RANS equations and two coupled second rank tensor equations for modeling the Reynolds stress ($\overline{u_i' u_j'}$). The model is often discussed in textbooks on advanced modeling of turbulent flows, but is rarely in use because of its complexity and because it is not implemented in any commercial CFD software. Without going too much into detail the most important equations of the model look something like

$$
\begin{aligned}
\frac{\partial \overline{u_i}}{\partial t} + \overline{u_j}\frac{\partial \overline{u_i}}{\partial x_j} &= -\frac{1}{\varrho}\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\nu(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}) - \frac{\partial \overline{u_i' u_j'}}{\partial x_j} + \overline{f_i}, \\
\frac{\partial \overline{u_i}}{\partial x_i} &= 0, \\
\frac{\partial \overline{u_i' u_j'}}{\partial t} + \overline{u_k}\frac{\partial \overline{u_i' u_j'}}{\partial x_k} + \frac{\partial T_{kij}}{\partial x_k} &= \mathbb{P}_{ij} + \mathbb{G}_{ij} - \varepsilon_{ij}, \\
L^2\nabla^2 f_{ij} - f_{ij} &= -\frac{\mathbb{C}_{ij}}{k} - \frac{\overline{u_i' u_j'}/k - 2\delta_{ij}/3}{T}, \\
\mathbb{P}_{ij} &= -\overline{u_i' u_k'}\frac{\partial \overline{u_j}}{\partial x_k} - \overline{u_j' u_k'}\frac{\partial \overline{u_i}}{\partial x_k}, \\
\varepsilon_{ij} &= 2\nu\overline{\frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k}}, \\
\mathbb{G}_{ij} &= \left(\varepsilon_{ij} - \frac{\overline{u_i' u_j'}}{k}\varepsilon\right) + k f_{ij}, \\
... &=
\end{aligned}
$$

Here $\overline{u_i}$ is a component of the Reynolds averaged velocity. The first two equations are basically the incompressible Navier-Stokes equations for $\overline{u_i}$ (with variable viscosity), while the rest of the equations define the turbulence model. Note that we have two PDEs for the two second rank tensors $\overline{u_i' u_j'}$ and f_{ij}. All in all the model requires solving for two second rank PDEs, one vector PDE and 3 scalar PDEs plus a number of derived quantities. That is, we need to solve 18 coupled, highly nonlinear PDEs.



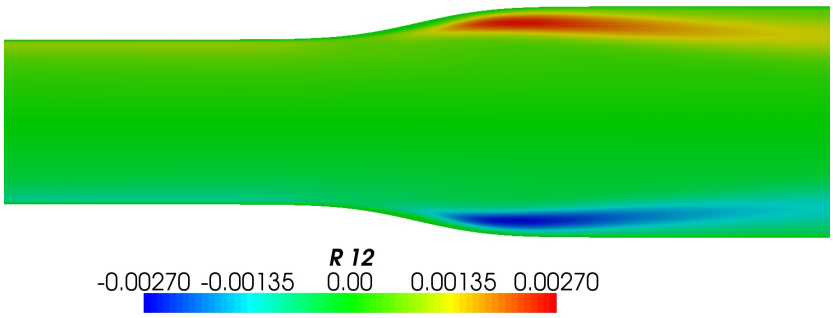
FEniCS has support for working with PDEs of second rank tensors and as such we have been able to implement the elliptic relaxation model using no more than 300 lines of code. The variational form for the two coupled second rank tensors looks like

```
class Steady_RijFij_1(RIJFIJBase):
    def form(self, Rij, Rij_, v_Rij, k_, e_, Pij_, nu, u_,
        nut_,
             Fij, Fij_, v_Fij, Aij_, Aij, PHIij_, Cmu, T_,
                 L_, **kwargs):
        Fr = nu*inner(nabla_grad(Rij),
            nabla_grad(v_Rij))*dx \
             + inner( dot(nabla_grad(Rij), u_) , v_Rij )*dx
                 \
             - inner( k_*Fij , v_Rij )*dx \
             - inner( Pij_ , v_Rij )*dx \
             + inner( Rij*e_*(1./k_) , v_Rij)*dx \
             + inner( Cmu*T_*dot(nabla_grad(Rij), Rij_),
                      nabla_grad(v_Rij) )*dx

        Ff = inner( nabla_grad(Fij),
            nabla_grad(L_**2*v_Fij) )*dx \
             + inner( Fij , v_Fij )*dx \
             - (1./k_)*inner( PHIij_ , v_Fij )*dx \
             - (2./T_)*inner( Aij_ , v_Fij )*dx

        return Fr + Ff
```

where `Rij`, `Fij`, `v_Rij`, and `v_Fij` are the trial- and test functions for $R_{ij} \equiv \overline{u_i' u_j'}$ and f_{ij}, respectively. The most recently computed approximations to `Rij` and `Fij` are recognized by an underscore: `Rij_` and `Fij_`. More details of the implementation and some results for turbulent flow in an axial diffusor is provided in `cbc.rans-MekIT11.pdf`. The contours of f_{12} (left) and $\overline{u_1' u_2'}$ (right) in the diffusior are shown below:



Nonlinear equations and linearization

One of the many advantages of using a high-level language like `FEniCS` for CFD is the ease of which we can experiment with various discretizations, coupling and linearizations of the same model. For example, all turbulence models are highly nonlinear and coupled with the Navier-Stokes equations. Nonlinear equations must be solved as a sequence of linear problems, but a standard linearization according to Newton's method will normally fail.

A feasible linearization, leading to a convergent iteration to solve the highly nonlinear equations, is not necessarily obvious for the turbulence model in question and usually calls for extensive trial and error. Using `cbc.pdesys`, the placement of a term in a variational form - explicitly on the right hand side of the equation system or implicitly in the coefficient matrix - is reduced to the inclusion or not of an underscore: `k` means an unknown finite element function k (`TrialFunction` object), while `k_` is the most recently computed approximation to `k` (`Function` object). For example, a nonlinear term k^2 can be linearized as `k_*k` or made fully known as `k_*k_`. The term can also be retained as `k*k` in a Newton method, where the corresponding Jacobian can be automatically computed.

As opposed to most other software packages for CFD, which require *user defined* PDEs to be solved in a segregated manner, the coupling or splitting of a system of PDEs is in `cbc.pdesys` a matter of inserting a few brackets in a little list. As a result, experimenting with numerics for complicated systems of nonlinear PDEs has never been easier!

Implementation details

There are basically three building blocks for setting up a problem with `cbc.pdesys`:

- `Problem` (defines the physical problem)

- `PDESystem` (defines a complete system of PDEs)
- `PDESubSystem` (defines one variational form as a subsystem of the complete system of PDEs)

Here we will briefly explain the rationale behind these three classes.

`PDESubSystem` is a class that contains all information necessary to assemble and solve one single variational form. In that way, a `PDESubSystem` is closely related to the `Linear/NonlinearVariationalProblem/Solver` classes provided with the regular Python `dolfin` package in FEniCS. In fact, all problems composed of one single variational form can equally well be set up with either approach, as demonstrated below. The `cbc.pdesys` package first shows its advantages when you need many variational forms to build your complete mathematical model of a physical phenomenon.

`PDESystem` is a class that contains a list of one or more `PDESubSystem` objects. For example, the Navier-Stokes equations can be represented through a `PDESystem` object. A coupled Navier-Stokes (NS) solver contains just one single `PDESubSystem`, which is a variational form for the coupled mixed finite element formulation for velocity and pressure. A segregated NS solver, on the other hand, contains two `PDESubSystem` objects, one for the velocity (vector field, governed by a vector PDE) and one for the pressure (scalar field, governed by a Poisson equation). The `PDESystem` object is responsible for creating all necessary `FunctionSpace`, `TestFunction`, and `TrialFunction` objects, as well as solution (`Function`) objects required to solve a certain system of PDEs.

`Problem` is a class that contains the mesh and boundaries (`SubDomain` objects), and that is responsible for initializing all `PDESystem` objects. The class also keeps track of any common parameters for all `PDESystem` objects, such as viscosity, time, and time step. Most importantly, the `Problem` class has implemented solve functionality used to advance any number of `PDESystem` objects simultaneously in time (or iterate over them in stationary problems).

Here is an example of how the Poisson equation can be solved, using either standard `dolfin` or `cbc.pdesys`:

```
from cbc.pdesys import *

mesh = UnitSquare(10, 10)
Q = FunctionSpace(mesh, 'CG', 1)
u = TrialFunction(Q)
v = TestFunction(Q)
u_ = Function(Q)
f = Constant(1.)
F = inner(nabla_grad(u), nabla_grad(v))*dx + f*v*dx
bcs = DirichletBC(Q, (0.), DomainBoundary())

# Implementation with LinearVariationalProblem/Solver
a, L = lhs(F), rhs(F)
poisson_problem = LinearVariationalProblem(a, L, u_,
    bcs=bcs)
poisson_solver  = LinearVariationalSolver(poisson_problem)
poisson_solver.solve()

```

```
# Implementation with cbc.pdesys
poisson = PDESubSystem(vars(), ['u'], bcs=[bcs], F=F)
poisson.solve()
```

Note that the `PDESubSystem` takes as argument the python namespace, `vars()`, containing the solution `Function`, `TrialFunction` etc. The reason for this choice will become more evident when the same problem is solved using both the `PDESystem` and `Problem` classes, where such objects are created automatically by `PDESystem`:

```
from cbc.pdesys import *

mesh = UnitSquare(10, 10)
# Change desired items in the problem_parameters dict from
    cbc.pdesys
problem = Problem(mesh, problem_parameters)
poisson = PDESystem([['u']], problem, solver_parameters)
poisson.setup() # Creates FunctionSpace, Functions etc.
poisson.f = Constant(1.)

class Poisson(PDESubSystem):
    def form(self, u, v_u, f, **kwargs):    # v_u is the
        TestFunction
        return inner(nabla_grad(u), nabla_grad(v_u))*dx +
            f*v_u*dx

bcs = DirichletBC(poisson.V['u'], (0.), DomainBoundary())
poisson.pdesubsystems['u'] = Poisson(vars(poisson), ['u'],
    bcs=[bcs])
problem.solve()
```

Here the namespace `vars(poisson)` contains `u`, `u_`, `v_u` (automatically created by `poisson.setup()`) and `f`. The namespace is futher provided as argument to the form method of the `Poisson` class.

Flow past a dolphin

We will now show a slightly more complicating example of how two `PDESystem` objects can be created and solved through the use of a `Problem` object. The physical problem regards the low Reynolds number flow past a hot two-dimensional dolphin (where of course the simplification to 2D eliminates any physical resemblance to an actual flow past an actual dolphin), where temperature (c) is modeled as a passive scalar with a nonlinear diffusion coefficient. The complete PDE system reads as follows in an appropriately scaled form,

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \nu\nabla^2\boldsymbol{u} - \nabla p + \boldsymbol{f}$$

$$\nabla\cdot\boldsymbol{u} = 0$$

$$\frac{\partial c}{\partial t} + \boldsymbol{u}\cdot\nabla c = \nabla\cdot\big(\nu(1+c^2)\nabla c\big)$$

Discretizing these equations with a Crank-Nicolson type of scheme in time, and redefining $\boldsymbol{u}$ to be the velocity at the new time level and $\boldsymbol{u}_1$ the velocity at the previous time level, we arrive at these spatial problems:

$$\frac{\boldsymbol{u}-\boldsymbol{u}_1}{\Delta t} + (\boldsymbol{u}_1\cdot\nabla)\boldsymbol{u}_1 = \nu\nabla^2\boldsymbol{U} - \nabla p + \boldsymbol{f}$$

$$\nabla\cdot\boldsymbol{U} = 0$$

$$\frac{c-c_1}{\Delta t} + \boldsymbol{U}\cdot\nabla C = \nabla\cdot\left(\nu(1+c^2)\nabla C\right),$$

with

$$\boldsymbol{U} = \frac{1}{2}\left(\boldsymbol{u}+\boldsymbol{u}_1\right), \quad C = \frac{1}{2}\left(c+c_1\right)$$

denoting the arithmetic averages needed in a Crank-Nicolson time integration. The corresponding variational formulation involves the integrals

$$\int_\Omega \left(\frac{\boldsymbol{u}-\boldsymbol{u}_1}{\Delta t}v_u + (\boldsymbol{u}_1\cdot\nabla\boldsymbol{u}_1)\cdot v_u + \nu\nabla\boldsymbol{U}\cdot\nabla v_u - p\nabla\cdot v_u - \boldsymbol{f}v_u + v_p\nabla\cdot\boldsymbol{U}\right)dx = 0,$$

$$\int_\Omega \left(\frac{c-c_1}{\Delta t}v_c + \boldsymbol{U}\cdot\nabla C + \nu(1+c^2)\nabla C\cdot\nabla v_c\right)dx = 0,$$

where v_u, v_p, and v_c are test functions for the test spaces for $\boldsymbol{u}$, p, and c, respectively.

The implementation of this model for the flow past a dolphin can be done as follows:

```
from cbc.pdesys import *

# Set up problem by loading mesh from file
mesh = Mesh('dolfin-outside.xml.gz')

# problem_parameters are defined in Problem.py
problem_parameters['time_integration'] = "Transient"    #
    default='Steady'
problem = Problem(mesh, problem_parameters)

# Set up first PDESystem
solver_parameters['space']['u'] = VectorFunctionSpace   #
    default=FunctionSpace
solver_parameters['degree']['u'] = 2                    #
    default=1
NStokes = PDESystem([['u', 'p']], problem,
    solver_parameters)
NStokes.setup()

# Use a constant forcing field to drive the flow from right
    to left
NStokes.f = Constant((-1., 0.))

# No-slip boundary condition for velocity on the dolfin
dolfin = AutoSubDomain(lambda x, on_boundary: on_boundary \
                       and not (near(x[0], 0) or near(x[0],
                           1.) or \
```

```
                        near(x[1], 0.) or near(x[1], 1.)))

bc = [DirichletBC(NStokes.V['up'].sub(0), Constant((0.0,
    0.0)), dolfin)]

# Set up variational form.
# u_, u_1, u_2 are the solution Functions at time steps N,
    N-1 and N-2.
# v_u/v_p are the TestFunctions for velocity/pressure in the
# MixedFunctionSpace for u and p

class NavierStokes(PDESubSystem):
    def form(self, u, v_u, u_, u_1, p, v_p, nu, dt, f, **
        kwargs):
        U = 0.5*(u + u_1)
        return (1./dt)*inner(u - u_1, v_u)*dx + \
               inner(u_1*nabla_grad(u_1), v_u) + \
               nu*inner(nabla_grad(U), nabla_grad(v_u))*dx -
                    \
               inner(div(v_u), p)*dx + v_p*div(U)*dx - \
               inner(f, v_u)*dx

NStokes.pdesubsystems['up'] = NavierStokes(
         vars(NStokes), ['u', 'p'], bcs=bc,
             reassemble_lhs=False)

# Integrate the solution from t=0 to t=0.5
problem.prm['T'] = 0.5
problem.solve()

# Define a new nonlinear PDESystem for a scalar c
scalar = PDESystem([['c']], problem, solver_parameters)
scalar.setup()

class Scalar(PDESubSystem):
    def form(self, c, v_c, c_, c_1, U_, dt, nu, **kwargs):
        C = 0.5*(c + c_1)
        return (1./dt)*inner(c - c_1, v_c)*dx + \
                inner(dot(U_, nabla_grad(C)), v_c)*dx + \
                nu*(1.+c_**2)*inner(nabla_grad(C),
                    nabla_grad(v_c))*dx
                # Note nonlinearity in c_ (above)

bcc = [DirichletBC(scalar.V['c'], Constant(1.0), dolfin)]

# Iterate on c_
scalar.U_ = 0.5*(NStokes.u_ + NStokes.u_1) # Scalar's form
    needs vel.
csub1 = Scalar(vars(scalar), ['c'], bcs=bcc,
    max_inner_iter=5)
scalar.pdesubsystems['c'] = csub1

# Integrate both PDESystems from t=0.5 to t=1.0 using Picard
# iterations on each time step
problem.prm['T'] = 1.0
problem.solve()

```

```
# Switch to using the Newton method for the nonlinear
    variational form
# With these calls we replace c by c_ in the Scalar form
    and compute
# the Jacobian wrt c_
csub1.prm['iteration_type'] = 'Newton'
csub1.define()

# Integrate both PDESystems from T=1.0 to T=1.5 using Newton
# iterations on each time step for the scalar
problem.prm['T'] = 1.5
problem.solve()
```

There are a few interesting features of `cbc.pdesys` at display here. First, in the creation of `NStokes` (`PDESystem` object), we request a coupled system of PDEs (using `MixedFunctionSpace`) consisting of the vector `u` and the scalar `p` (scalar is default option). A segregated system, on the other hand, would require the list `[['u'], ['p']]` being sent to the `PDESystem` object to indicate that `u` and `p` are solved in sequence, i.e., in a segregated way. The `solver_parameters` dictionary contains many dictionaries, with default values for many of the options. The dictionaries use the names of the variables (here `u` and `p`) as keys. `FunctionSpace` is the default option for the `space` dictionary and `1` for the `degree` dictionary (polynomial order of the basis functions), and as such we need only specify new values for `u`.

The variational form is hooked up by subclassing the `PDESubSystem` class and overloading the `form` method that returns the variational form. The `PDESubSystem` class contains numerous methods and switches for optimization of finite element assembly and solving linear or nonlinear system arising from the form. Since the Navier-Stokes equations being solved here are discretized with explicit convection, the left hand side coefficient matrix will not change in time. When we provide this information (through `reassemble_lhs=False`), the coefficient matrix will only be assembled on the first time step.

One major advantage of placing numerical schemes as methods in a variational form class is the ease of which we can manipulate and store numerous different discretizations. The classes of numerical schemes are typically kept in a single file, or Python module (e.g., `NavierStokes.py`), and can be retrieved as required. So if we in the future need to solve the Navier-Stokes equations together with other PDEs, then we can simply pull the scheme from `NavierStokes.py` and reuse it. This is not possible with the standard `dolfin` implementation displayed above. For turbulent flow models, we would like to set up our problem and then select the appropriate turbulence model and numerics from a predefined library. Each turbulence model will then have a main `PDESystem` class and a library of possible transient and steady schemes that can be picked at runtime.

Note that implementing a new problem through `cbc.pdesys` generally will not require redefining the variational forms as done above (`Scalar` and `NavierStokes`). Instead the user will be required to set up a mesh and its boundaries, pick

`PDESystem's` from modules, initialize and solve. In the end this leads to very compact, flexible and, most importantly, reusable code.

RANS models

Most industrial flows have high Reynolds number and are far too complex for all details of the flow to be fully resolved. For this reason researchers have developed simplified models representing the most relevant statistical properties of the flow, like the mean velocity and the mean turbulent kinetic energy. The largest family of such models are the Reynolds Averaged Navier Stokes (RANS) equations. There are hundreds of different RANS models, each represented by a system of nonlinear PDEs, coupling statistical turbulence quantities with the mean flow.

There is a hierarchy of turbulence models. So-called eddy-viscosity (EV) models close the Reynolds stress through the following formula:

$$\overline{u_i' u_j'} = -\nu_T \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) + \frac{1}{3} \delta_{ij} \overline{u_k' u_k'}$$

Eddy-viscosity models are usually classified by the number of additional PDEs that are required to close an expression for the turbulent viscosity ν_T. Reynolds stress models, like the elliptic relaxation model outlined above, solves a PDE for the second rank tensor $\overline{u_i' u_j'}$ and do not make use of the eddy-viscosity model. Using `cbc.pdesys` we have currently implemented the following turbulence models in `cbc.rans`:

1. One-equation EV models
    - Spalart-Allmaras
2. Two-equation EV models
    - Standard k-epsilon
    - Low-Reynolds k-epsilon (3 different)
    - Menter's SST
3. Four-equation EV models
    - V2F (2 different)
4. Reynolds stress models
    - Standard
    - Elliptic relaxation

The tutorial cbc.rans-MekIT11.pdf on using cbc.rans to implement advanced turbulence models was published in the proceedings of the 6th National Conference on Computational Mechanics, 2011 (MekIT'11).

The interested reader will also learn more about the motivation for, the design, and the inner workings of the cbc.rans package by studying the recently published paper A FEniCS-Based Programming Framework for Modeling Turbulent Flow by the Reynolds-Ave (*Advances in Water Resources*, 2011, DOI: 10.1016/j.advwatres.2011.02.013).