reactionsystem_solution

April 6, 2022

1 Problem

We solve a reaction diffusion advection problem involving three species with a given velocity field. The stream function ψ for the velocity field is hereby the solution to the Laplace-equation:

$$
\begin{aligned}
-\Delta\psi = 0.8\pi 2\sin(2\pi x)\sin(2\pi y) \quad \text{in } \Omega = [0,1]^2, \\
\psi = 0 \quad \text{on } \partial\Omega.
\end{aligned}
$$

With that the velocity field is given by

$$
w = (-\partial_y\psi, \partial_x\psi) \tag{1}
$$

The three species $u = (u_0, u_1, u_2)$ satisfy the PDE:

$$
\int_\Omega \frac{u^{n+1} - u^n}{\Delta t} v + K(\nabla u^{n+1})\nabla u^{n+1} \cdot \nabla v \; dx = \int_\Omega f(x, t^n + \Delta t) v \; dx + \int_{\partial\Omega} g(x, t^n + \Delta t) \cdot n \; v \; ds \; .
$$

where S describes some source or sink and the reaction term is given by

$$
R(u) = K(-u_0 u_1, -u_0 u_1, 2u_0 u_1 - 10u_2)^T \tag{2}
$$

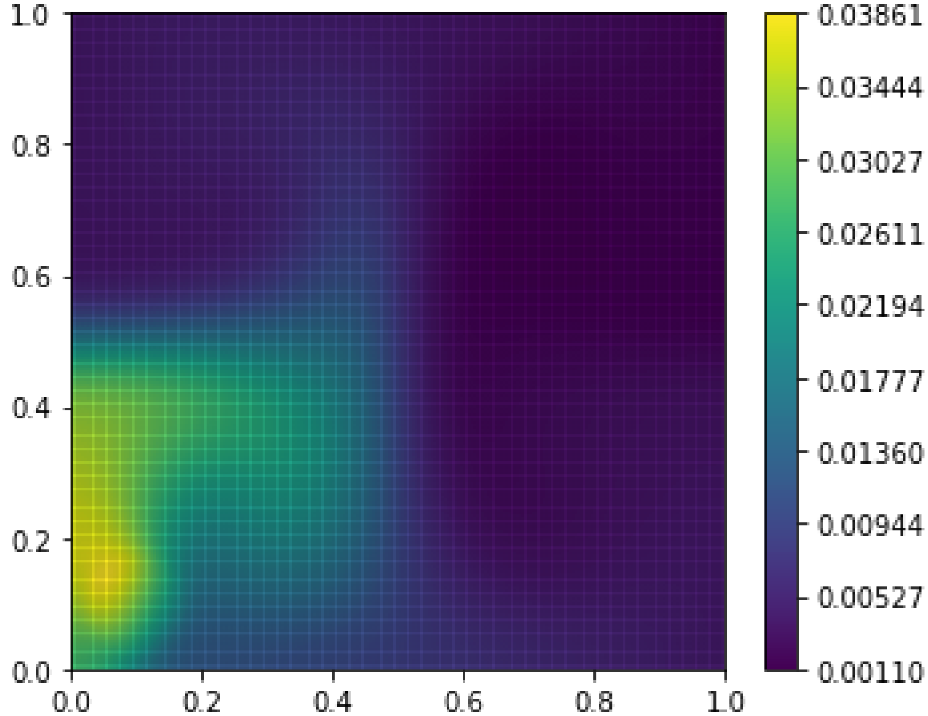
where K is a reaction coefficient.

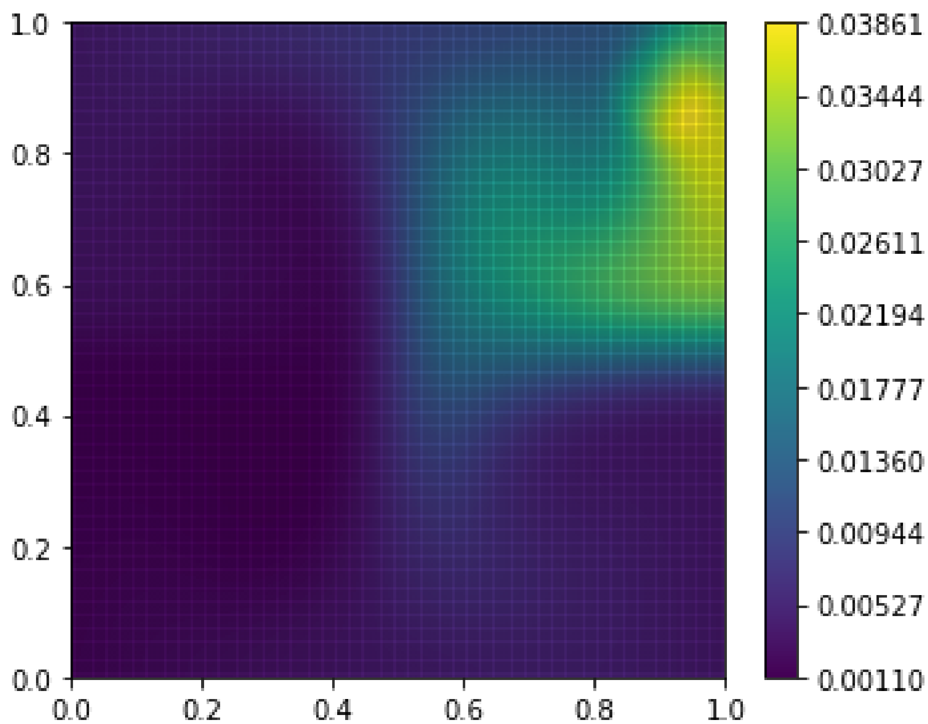
[1]:
```
import math
import ufl
from ufl import grad, div, dot, dx, inner, sin, cos, pi
import dune.ufl
import dune.grid
import dune.fem

endTime  = 5
saveInterval = 0.5

gridView = dune.grid.structuredGrid([0,0],[1,1],[100,100])

# Define stream-function and transport field w
# analytic:
```

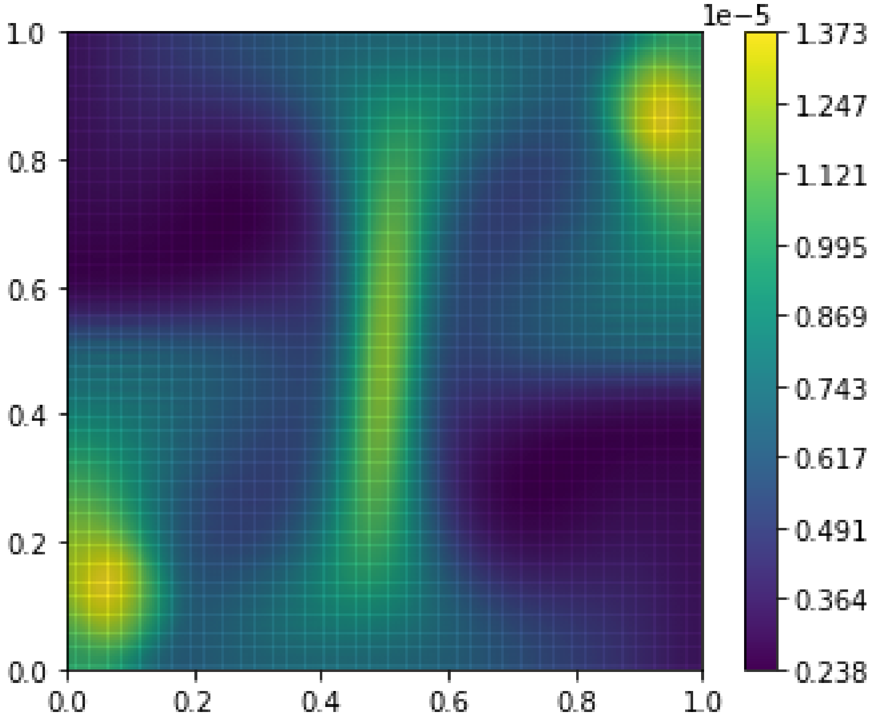
```
# Psi     = 0.1*sin(2*pi*x[0])*sin(2*pi*x[1])
# discrete:
velocitySpace = dune.fem.space.lagrange(gridView, order=1)
Psi  = velocitySpace.interpolate(0,name="stream_function")
u    = ufl.TrialFunction(velocitySpace)
phi  = ufl.TestFunction(velocitySpace)
x    = ufl.SpatialCoordinate(velocitySpace)
form = ( inner(grad(u),grad(phi)) -
         0.1*2*(2*pi)**2*sin(2*pi*x[0])*sin(2*pi*x[1]) * phi ) * dx
dbc  = dune.ufl.DirichletBC(velocitySpace,0)
velocityScheme = dune.fem.scheme.galerkin([form == 0, dbc], solver="cg")
velocityScheme.solve(target=Psi)
w       = ufl.as_vector([-Psi.dx(1),Psi.dx(0)])

space = dune.fem.space.lagrange(gridView, order=1, dimRange=3)
u     = ufl.TrialFunction(space)
phi   = ufl.TestFunction(space)
x     = ufl.SpatialCoordinate(space)

# reaction, diffusion and other coefficients
K   = dune.ufl.Constant(10.0, "reactionRate")
eps = dune.ufl.Constant(0.01, "diffusionRate")
dt  = dune.ufl.Constant(0.01, "dt")
Q   = dune.ufl.Constant(0.1, "sourceStrength")

# define storage for discrete solutions
uh     = space.interpolate([0,0,0], name="uh")
uh_old = uh.copy()

# define source terms
P1 = ufl.as_vector([0.1,0.1])
P2 = ufl.as_vector([0.9,0.9])
RF = 0.075
f1 = ufl.conditional(dot(x-P1,x-P1) < RF**2, Q, 0)
f2 = ufl.conditional(dot(x-P2,x-P2) < RF**2, Q, 0)
f  = ufl.as_vector([f1,f2,0])

# reaction rates
r   = K*ufl.as_vector([u[0]*u[1], u[0]*u[1], -2*u[0]*u[1] + 10*u[2]])

xForm = (dot(grad(u)*w + r - f, phi) + eps * inner(grad(u), grad(phi))) * dx
form  = dot(u - uh_old, phi) * dx + dt * xForm

scheme = dune.fem.scheme.galerkin(form == 0, solver="gmres")

nextSaveTime = saveInterval
```

```
vtk = gridView.sequencedVTK("reactionsystem", pointdata=[uh],␣
↪pointvector={"velocity":w})
vtk()

# set time step size
scheme.model.dt = 0.01

scheme.model.reactionRate  = 10.
scheme.model.diffusionRate = 0.01
scheme.model.sourceStrength = 0.1

t = 0
while t < endTime:
    uh_old.assign(uh)
    info = scheme.solve(target=uh)
    t += dt.value
    if t >= nextSaveTime or t >= endTime:
        print("Computed solution at time",t,\
              "iterations: ", info["linear_iterations"], "#elem: ", gridView.
↪size(0) )
        vtk()
        nextSaveTime += saveInterval

uh[0].plot()
uh[1].plot()
uh[2].plot()
```

```
Computed solution at time 0.5000000000000002 iterations:  5 #elem:  10000
Computed solution at time 1.0000000000000007 iterations:  4 #elem:  10000
Computed solution at time 1.500000000000001 iterations:  3 #elem:  10000
Computed solution at time 2.0000000000000013 iterations:  3 #elem:  10000
Computed solution at time 2.5099999999999905 iterations:  4 #elem:  10000
Computed solution at time 3.00999999999998 iterations:  4 #elem:  10000
Computed solution at time 3.509999999999969 iterations:  4 #elem:  10000
Computed solution at time 4.009999999999959 iterations:  3 #elem:  10000
Computed solution at time 4.509999999999948 iterations:  3 #elem:  10000
Computed solution at time 5.009999999999938 iterations:  3 #elem:  10000
```


0.03861
0.03444
0.03027
0.02611
0.02194
0.01777
0.01360
0.00944
0.00527
0.00110
0.0
0.2
0.4
0.6
0.8
1.0


0.03861
0.03444
0.03027
0.02611
0.02194
0.01777
0.01360
0.00944
0.00527
0.00110
0.0
0.2
0.4
0.6
0.8
1.0


1e−5
1.373
1.247
1.121
0.995
0.869
0.743
0.617
0.491
0.364
0.238
0.0
0.2
0.4
0.6
0.8
1.0