

# Mathematical Modelling and Simulation with Comsol Multiphysics II

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## Exercise 3

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**Bearbeitung: Montag, 26.10.2015, 12:30-14:00 Uhr** (während der Übung).

### Exercise 3 (Quintic Nagumo equation: Traveling Wave).

Consider the **quintic Nagumo equation**

$$u_t = u_{xx} + u(1-u)(u-\alpha_1)(u-\alpha_2)(u-\alpha_3), \quad x \in \mathbb{R}, t \geq 0$$

for some  $\alpha_1, \alpha_2, \alpha_3 \in (0, 1)$  with  $\alpha_1 < \alpha_2 < \alpha_3$  and  $u = u(x, t) \in \mathbb{R}$ .

a) Solve the **nonfrozen quintic Nagumo equation**

$$(1) \quad \begin{aligned} u_t &= u_{xx} + u(1-u)(u-\alpha_1)(u-\alpha_2)(u-\alpha_3) & , x \in \Omega, t \in (0, T_1], \\ u(0) &= u_0 & , x \in \bar{\Omega}, t = 0, \\ u_x &= 0 & , x \in \partial\Omega, t \in [0, T_1], \end{aligned}$$

on the spatial domain  $\Omega = [-100, 100]$  for end time  $T_1 = 1500$ , initial data  $u_0(x) = \frac{\tanh(x)+1}{2}$  and parameters  $\alpha_1 = \frac{2}{5}$ ,  $\alpha_2 = \frac{1}{2}$ ,  $\alpha_3 = \frac{17}{20}$ . For the space discretization use linear Lagrange elements with maximal element size  $\Delta x = 0.3$ . For the time discretization use the BDF method of maximum order 2 with intermediate time steps, time stepsize  $\Delta t = 0.3$ , relative tolerance  $\text{rtol} = 10^{-2}$  and absolute tolerance  $\text{atol} = 10^{-3}$  with global method set to be unscaled. The nonlinear equations should be solved by the Newton method. i.e. automatic (Newton).

Follow the steps below to realize the implementation:

1. **Model Wizard**: Choose space dimension '1D', create a 'Coefficient Form PDE' with dependent variable 'u' and select a 'time-dependent' study.
2. **Geometry**: Build the spatial domain  $\Omega = [-100, 100]$ .
3. **Equation settings**: Implement the PDE, the initial data and the boundary conditions. Choose the shape functions for spatial discretization.
4. **Parameters and Variables**: Define the (global) parameter  $\alpha_1 = \frac{2}{5}$ ,  $\alpha_2 = \frac{1}{2}$ ,  $\alpha_3 = \frac{17}{20}$  and the (local) variables  $u_0 = \frac{\tanh(x)+1}{2}$  and  $fu = u(1-u)(u-\alpha_1)(u-\alpha_2)(u-\alpha_3)$ .
5. **Mesh**: Build a user-controlled mesh with maximal element size  $\Delta x = 0.3$ .
6. **Study 1**: Create a time-dependent study ('Study 1, Step 1') for  $t$  from 0 to 1500 with stepsize  $\Delta t = 0.3$  and relative tolerance  $\text{rtol} = 10^{-2}$ . In the solver settings choose absolute tolerance  $\text{atol} = 10^{-3}$  with global method set to be unscaled, BDF method of maximum order 2 with intermediate time steps and the Newton method for the nonlinear solver. Create a solution store for the solution of (1).

b) Solve the **frozen quintic Nagumo equation**

$$(2) \quad \begin{aligned} v_t &= v_{\xi\xi} + \mu v_{\xi} + v(1-v)(v-\alpha_1)(v-\alpha_2)(v-\alpha_3) & , \xi \in \Omega, t \in (0, T_2], \\ v(0) &= v_0 & , \xi \in \bar{\Omega}, t = 0, \\ v_{\xi} &= 0 & , \xi \in \partial\Omega, t \in [0, T_2], \\ 0 &= (v - \hat{v}, \hat{v}_x)_{L^2(\Omega, \mathbb{R})} & , t \in [0, T_2], \\ \gamma_t &= \mu & , t \in (0, T_2], \\ \gamma(0) &= 0 & , t = 0 \end{aligned}$$

on the spatial domain  $\Omega = [-100, 100]$  for end time  $T_2 = 3000$ , initial data  $v_0(\xi) = u_0(\xi)$ , reference function  $\hat{v}(\xi) = u_0(\xi)$  and parameters  $\alpha_1 = \frac{2}{5}$ ,  $\alpha_2 = \frac{1}{2}$ ,  $\alpha_3 = \frac{17}{20}$ . For the space discretization use linear Lagrange elements with maximal element size  $\Delta x = 0.3$ . For the time discretization use the BDF method of maximum order 2 with intermediate time steps, time stepsize  $\Delta t = 0.3$ , relative tolerance  $\text{rtol} = 10^{-3}$  and absolute tolerance  $\text{atol} = 10^{-4}$  with global method set to be unscaled. The nonlinear equations should be solved by the Newton method (automatic (Newton)).

To realize the implementation, extend your model from a) as follows:

7. **Model Wizard:** Add a 'Coefficient Form PDE' with dependent variable 'v' and two 'Weak Form Boundary PDE' with dependent variable 'mu' and 'g' for a 'time-dependent' study.
8. **Equation settings:** Implement the PDE, the initial data and the boundary conditions. Choose the shape functions for spatial discretization.
9. **Equation settings:** Implement the weak form boundary for 'mu' using the weak form 'test(mu1)\*pc1'. This equation has to be stated only in the left boundary point. Choose the shape functions for spatial discretization.
10. **Equation settings:** Implement the weak form boundary for 'g' using the weak form 'test(g1)\*mu1'. This equation has to be stated only in the left boundary point. Choose the shape functions for spatial discretization.
11. **Variables:** Extend the (local) variables ('Variables 1') by defining 'fv=v\*(1-v)\*(v-alpha1)\*(v-alpha2)\*(v-alpha3)', 'Fv=mu1cpl\*vx+fv', 'v0=u0', 'vh=u0' and 'pc1\_fix=d(vh,x)\*(v-vh)'.
12. **Integration operators:** Define an integration operator 'intop1', that integrates an expression over the domain with integration order 2. Further, define an integration operator 'intop2', that integrates an expression over the left boundary point with integration order 1.
13. **Expressions to integrate:** Define (local) variables ('Variables 2') containing the expressions for domain integration, i.e. variable 'intcpl\_source\_pc1' with expression 'pc1\_fix' and variable 'intcpl\_source\_sqr\_vt' with expression 'vt^2'.
14. **Expressions to integrate:** Define (local) variables ('Variables 3') containing the expressions for boundary integration, i.e. variable 'intcpl\_source\_mu1cpl' with expression 'mu1'.
15. **Variables for results of integration:** Define (global) variables ('Variables 4') containing the result of integration, i.e. variable 'pc1' with expression 'comp1.intop1(intcpl\_source\_pc1)', variable 'sqr\_vt' with expression 'comp1.intop1(intcpl\_source\_sqr\_vt)' and variable 'mu1cpl' with expression 'comp1.intop1(intcpl\_source\_mu1cpl)'.
16. **Study 2:** Create a time-dependent study ('Study 2, Step 1') for  $t$  from 0 to 3000 with stepsize  $\Delta t = 0.3$  and relative tolerance  $\text{rtol} = 10^{-3}$ . In the solver settings choose absolute tolerance  $\text{atol} = 10^{-4}$  with global method set to be unscaled, BDF method of maximum order 2 with intermediate time steps and the Newton method for the nonlinear solver. Create a solution store for the solution of (2).

c) Solve the **eigenvalue problem** for the linearization of the quintic Nagumo equation

$$(3) \quad \begin{aligned} \lambda w &= w_{\xi\xi} + \mu_{\star} w_{\xi} + f'(v_{\star})w & , \xi \in \Omega, \\ w_{\xi} &= 0 & , \xi \in \partial\Omega \end{aligned}$$

on the spatial domain  $\Omega = [-100, 100]$ , where  $f'(v)$  denotes the derivative of

$$f(v) = v(1 - v)(v - \alpha_1)(v - \alpha_2)(v - \alpha_3).$$

For  $v_*$  and  $\mu_*$  use the solutions  $v$  and  $\mu$  of (2) at the end time  $T_2 = 3000$ . Determine  $\text{neigs} = 400$  eigenvalues  $\lambda$  and corresponding eigenfunctions  $w$ . The eigenvalues should be closest in absolute value around the shift  $-1$ .

To realize the implementation, extend your model from b) as follows:

17. **Study 2:** Create 'Compile Equations', 'Dependent Variables' and 'Eigenvalue Solver' for 'Solution 3'. Build a further study step ('Study 1, Step 2') 'Eigenvalue' study. In the eigenvalue solver settings choose the number of eigenvalues  $\text{neigs} = 400$ , the shift  $-1$  and the eigenvalue search method. Define the linearization point and the values of variables not solved for to be the solution of (2) at the end time  $T_2$ . Create a solution store for the solution of (3).

d) **Postprocessing and Visualization** of results: Create the following plots to visualize the results of the computations:

- **Traveling Front, View 1:** Plot the solution  $u$  of (1) at the time instances  $t = 400, 800$  and  $1200$ .
- **Traveling Front, View 2:** Create a time-space plot for the solution  $u$  of (1).
- **Profile, View 1:** Plot the solution  $v$  of (2) at the end time  $T_2$ .
- **Profile, View 2:** Create a time-space plot for the solution  $v$  of (2).
- **Velocity:** Plot the velocity  $mu$  of (2) for time  $t$  from  $0$  to  $T_2$ .
- **Position:** Plot the position  $g$  of (2) for time  $t$  from  $0$  to  $T_2$ .
- **Reference function:** Plot the template  $vh$ .
- **Convergence indicator:** Plot  $\|v_t(t)\|_{L^2(\Omega, \mathbb{R})}$  and  $|\mu_t(t)|$  for time  $t$  from  $0$  to  $T_2$ .
- **Eigenvalues and Spectrum:** Plot the eigenvalues  $\lambda$  of (3).
- **Eigenfunctions:** Plot the eigenfunction  $w$  of (3) belonging to the zero eigenvalue.