Mathematical Modelling and Simulation with Comsol Multiphysics II
Winter term 2015/2016
Exercise 7
Dr. Denny Otten

Bearbeitung: Montag, 16.11.2015, 12:30-14:00 Uhr (während der Übung).

Exercise 7 (Gross-Pitaevskii equation: Oscillating pulse).
Consider the **Gross-Pitaevskii equation**

$$u_t = \alpha \triangle u + \beta |u|^2 u + \gamma V(x) u, \quad x \in \mathbb{R}^d,\, t \geqslant 0 \tag{1}$$

for some $\alpha,\beta,\gamma \in \mathbb{C}$ with $\alpha = \frac{i}{2}$, $V : \mathbb{R}^d \to \mathbb{R}$ and $u = u(x,t) \in \mathbb{C}$. In a)-d), we implement the real-valued version of (1): Decomposing

$$u = u_1 + i u_2, \quad \alpha = a_1 + i a_2, \quad \beta = b_1 + i b_2, \quad \gamma = c_1 + i c_2$$

with $u_1, u_2, a_1, a_2, b_1, b_2, c_1, c_2 \in \mathbb{R}$ and introducing

$$A = \begin{pmatrix} a_1 & -a_2 \\ a_2 & a_1 \end{pmatrix}, \quad B = \begin{pmatrix} b_1 & -b_2 \\ b_2 & b_1 \end{pmatrix}, \quad C = \begin{pmatrix} c_1 & -c_2 \\ c_2 & c_1 \end{pmatrix}, \quad u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

with $A, B, C \in \mathbb{R}^{2,2}$ and $u = u(x,t) \in \mathbb{R}^2$ the real-valued system associated with (1) reads as

$$u_t = A \triangle u + B |u|^2 u + C V(x) u, \quad x \in \mathbb{R}^d,\, t \geqslant 0.$$

a) Consider the one-dimensional **nonfrozen Gross-Pitaevskii equation**

$$\begin{aligned} u_t &= \alpha u_{xx} + \beta |u|^2 u + \gamma V(x) u &&, x \in \Omega,\, t \in (0,T_1], \\ u(0) &= u_0 &&, x \in \bar{\Omega},\, t = 0, \\ u_x &= 0 &&, x \in \partial\Omega,\, t \in [0,T_1], \end{aligned} \tag{2}$$

Solve the real-valued system associated with (2)

$$\begin{aligned} u_t &= A u_{xx} + B |u|^2 u + C V(x) u &&, x \in \Omega,\, t \in (0,T_1], \\ u(0) &= u_0 &&, x \in \bar{\Omega},\, t = 0, \\ u_x &= 0 &&, x \in \partial\Omega,\, t \in [0,T_1], \end{aligned} \tag{3}$$

on the spatial domain $\Omega = (-10, 10)$ for end time $T_1 = 80$, initial data $u_0 = (u_0^{(1)}, u_0^{(2)})^T$ with $u_0^{(1)}(x) = \pi^{-\frac{1}{4}} \exp\left(-\frac{x^2}{2}\right)$, $u_0^{(2)}(x) = 0$ and parameters $\alpha = \frac{i}{2}$, $\beta = -i$, $\gamma = -i$ and $V(x) = \frac{x^2}{2}$. For the space discretization use linear Lagrange elements with maximal element size $\triangle x = 0.05$. For the time discretization use the BDF method of maximum order 2 with intermediate time steps, time stepsize $\triangle t = 0.1$, relative tolerance rtol $= 10^{-2}$ and absolute tolerance atol $= 10^{-4}$ with global method set to be unscaled. The nonlinear equations should be solved by the Newton method. i.e. automatic (Newton).

b) Consider the one-dimensional **nonfrozen Gross-Pitaevskii equation**

$$\begin{aligned} \hat{v}_t &= \alpha \hat{v}_{xx} + \beta |\hat{v}|^2 \hat{v} + \gamma V(x) \hat{v} &&, x \in \Omega,\, t \in (0,T_2], \\ \hat{v}(0) &= \hat{v}_0 &&, x \in \bar{\Omega},\, t = 0, \\ \hat{v}_x &= 0 &&, x \in \partial\Omega,\, t \in [0,T_2], \end{aligned} \tag{4}$$

Solve the real-valued system associated with (4)

$$
(5)\qquad
\begin{aligned}
\hat{v}_t &= A\hat{v}_{xx} + B|\hat{v}|^2\hat{v} + CV(x)\hat{v} &&, x \in \Omega,\ t \in (0,T_2],\\
\hat{v}(0) &= \hat{v}_0 &&, x \in \bar{\Omega},\ t = 0,\\
\hat{v}_x &= 0 &&, x \in \partial\Omega,\ t \in [0,T_2],
\end{aligned}
$$

on the spatial domain $\Omega = (-10, 10)$ for end time $T_2 = 1$, initial data $\hat{v}_0(x) = u_0(x)$ and parameters $\alpha = \frac{i}{2}$, $\beta = -i$, $\gamma = -i$ and $V(x) = \frac{x^2}{2}$. For the space discretization use linear Lagrange elements with maximal element size $\triangle x = 0.05$. For the time discretization use the BDF method of maximum order 2 with intermediate time steps, time stepsize $\triangle t = 0.1$, relative tolerance rtol $= 10^{-2}$ and absolute tolerance atol $= 10^{-4}$ with global method set to be unscaled. The nonlinear equations should be solved by the Newton method. i.e. automatic (Newton).

c) Consider the **frozen Gross-Pitaevskii equation**

$$
(6)\qquad
\begin{aligned}
v_t &= \alpha v_{\xi\xi} + i\mu v + \beta|v|^2 v + \gamma V(x)v &&, \xi \in \Omega,\ t \in (0,T_3],\\
v(0) &= v_0 &&, \xi \in \bar{\Omega},\ t = 0,\\
v_\xi &= 0 &&, \xi \in \partial\Omega,\ t \in [0,T_3],\\
0 &= \mathrm{Re}\,(v - \hat{v}, i\hat{v})_{L^2(\Omega,\mathbb{C})} &&, t \in [0,T_3],\\
\gamma_t &= \mu &&, t \in (0,T_3],\\
\gamma(0) &= 0 &&, t = 0
\end{aligned}
$$

Solve the real-valued system associated with (6)

$$
(7)\qquad
\begin{aligned}
v_t &= Av_{\xi\xi} + \mu S_2 v + B|v|^2 v + CV(x)v &&, \xi \in \Omega,\ t \in (0,T_3],\\
v(0) &= v_0 &&, \xi \in \bar{\Omega},\ t = 0,\\
v_\xi &= 0 &&, \xi \in \partial\Omega,\ t \in [0,T_3],\\
0 &= (v - \hat{v}, S_2\hat{v})_{L^2(\Omega,\mathbb{R}^2)} &&, t \in [0,T_3],\\
\gamma_t &= \mu &&, t \in (0,T_3],\\
\gamma(0) &= 0 &&, t = 0
\end{aligned}
$$

on the spatial domain $\Omega = (-10, 10)$ for end time $T_3 = 200$, initial data $v_0(\xi) = u_0(\xi)$, reference function $\hat{v}(\xi)$ as the solution of (5) at end time T_2 and parameters $\alpha = \frac{i}{2}$, $\beta = -i$, $\gamma = -i$, $V(x) = \frac{x^2}{2}$ and $S_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. For the space discretization use linear Lagrange elements with maximal element size $\triangle x = 0.05$. For the time discretization use the BDF method of maximum order 2 with intermediate time steps, time stepsize $\triangle t = 0.5$, relative tolerance rtol $= 10^{-2}$ and absolute tolerance atol $= 10^{-3}$ with global method set to be unscaled. The nonlinear equations should be solved by the Newton method (automatic (Newton)).

d) Solve the **eigenvalue problem** for the linearization of the real-valued version of the Gross-Pitaevskii equation

$$
(8)\qquad
\begin{aligned}
\lambda w &= Aw_{\xi\xi} + \mu_\star S_2 w + D_v f(v_\star)w &&, \xi \in \Omega,\\
w_\xi &= 0 &&, \xi \in \partial\Omega
\end{aligned}
$$

on the spatial domain $\Omega = (-10, 10)$, where $D_v f(v)$ denotes the derivative of

$$
f(v) = B|v|^2 v + CV(x)v, \text{ i.e. } D_v f(v) = B|v|^2 + 2Bvv^T + CV(x).
$$

For $v_\star$ and $\mu_\star$ use the solutions v and μ of (7) at the end time $T_2 = 200$. Determine neigs $= 400$ eigenvalues λ and correspondig eigenfunctions w. The eigenvalues should be closest in absolute value around the shift -1.

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

 - Oscillating Pulse, View 1: Plot the solution u_1 of (3) at time $t = 0, 2, 3, 4$ and 8.
 - Oscillating Pulse, View 1: Plot the solution u_2 of (3) at time $t = 0, 2, 3, 4$ and 8.
 - Oscillating Pulse, View 2: Create a time-space plot for the solution u_1 of (3).
 - Oscillating Pulse, View 2: Create a time-space plot for the solution u_2 of (3).
 - Reference function: Plot the template solutions $\hat{v}_1$ and $\hat{v}_2$ of (5) at time $T2$.
 - Profile, View 1: Plot the solution v_1 and v_2 of (7) at the end time T_3.
 - Profile, View 2: Create a time-space plot for the solution v_1 of (7).
 - Profile, View 2: Create a time-space plot for the solution v_2 of (7).
 - Velocity: Plot the velocity μ of (7) for time t from 0 to T_3.
 - Position: Plot the position γ of (7) for time t from 0 to T_3.
 - Convergence indicator: Plot $\|v_t(t)\|_{L^2(\Omega,\mathbb{R}^2)}$ and $|\mu_t(t)|$ for time t from 0 to T_3.
 - Eigenvalues and Spectrum: Plot the eigenvalues λ of (8).
 - Eigenfunctions: Plot the eigenfunction w of (8) belonging to the zero eigenvalue.