1 Introduction

Let $\Omega \subseteq \mathbb{R}^n$, $V : \Omega \to \mathbb{R}$, $\kappa \in \mathbb{R}$, and $\psi : (0,T) \times \Omega \to \mathbb{C}$. The Nonlinear Schroedinger Equation (NSE) is given by:

$$-\mathrm{i}\frac{\partial \psi}{\partial t} - \frac{1}{2}\Delta\psi + V\psi + \kappa|\psi|^2\psi = 0$$

With initial conditions:

$$\psi(0, \boldsymbol{x}) = \psi_0(\boldsymbol{x})$$

For all $\boldsymbol{x} \in \Omega$ and with boundary conditions:

$$\psi(t, \boldsymbol{x}) = 0$$

For all $(t, \boldsymbol{x}) \in (0,T) \times \partial\Omega$.

Because ψ is complex-valued, it is convenient to separate the equation into real and imaginary parts. If we take $\psi(t, \boldsymbol{x}) = u(t, \boldsymbol{x}) + \mathrm{i}v(t, \boldsymbol{x})$ for $u, v : (0,T) \times \Omega \to \mathbb{R}$, we also have that $|\psi|^2 = u^2 + v^2$:

$$-\mathrm{i}\frac{\partial}{\partial t}(u + \mathrm{i}v) - \frac{1}{2}\Delta(u + \mathrm{i}v) + V(u + \mathrm{i}v) + \kappa(u^2 + v^2)(u + \mathrm{i}v) = 0$$

So:

$$\begin{aligned} \frac{\partial v}{\partial t} - \frac{1}{2}\Delta u + Vu + \kappa(u^2 + v^2)u = 0 \\ -\frac{\partial u}{\partial t} - \frac{1}{2}\Delta v + Vv + \kappa(u^2 + v^2)v = 0 \end{aligned}$$

2 Toy Problem

Let $\Omega = [-1, 1]^n$, and consider, for an example:

$$u(t, \boldsymbol{x}) = \cos(\pi t) \prod_{i=1}^{n} \cos(\pi x_i)$$
$$v(t, \boldsymbol{x}) = \sin(\pi t) \prod_{i=1}^{n} \cos(\pi x_i)$$

Then:

$$u(0, \boldsymbol{x}) = \prod_{i=1}^{n} \cos(\pi x_i)$$
$$v(0, \boldsymbol{x}) = 0$$

We have that:

$$\begin{aligned} u^2 + v^2 &= \cos^2(\pi t) \prod_{i=1}^{n} \cos^2(\pi x_i) + \sin^2(\pi t) \prod_{i=1}^{n} \cos^2(\pi x_i) \\ &= (\cos^2(\pi t) + \sin^2(\pi t)) \prod_{i=1}^{n} \cos^2(\pi x_i) \\ &= \prod_{i=1}^{n} \cos^2(\pi x_i) \end{aligned}$$

Note that $u^2 + v^2$ is independent of t. So:

Meanwhile:

$$\begin{aligned} \frac{\partial u}{\partial x_k} &= -\pi \cos(\pi t) \sin(\pi x_k) \prod_{i \neq k} \cos(\pi x_i) \\ \frac{\partial^2 u}{\partial x_k^2} &= -\pi^2 \cos(\pi t) \prod_{i=1}^{n} \cos(\pi x_i) \\ &= -\pi^2 u \\ \Delta u &= \sum_{k=1}^{n} \frac{\partial^2 u}{\partial x_k^2} \\ &= -n\pi^2 u \end{aligned}$$

Similarly:

$$\Delta v = -n\pi^2 v$$

And:

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= -\pi \sin(\pi t) \prod_{i=1}^{n} \cos(\pi x_i) \\
&= -\pi v \\
\frac{\partial v}{\partial t} &= \pi \cos(\pi t) \prod_{i=1}^{n} \cos(\pi x_i) \\
&= \pi u
\end{aligned}
$$

Then, rewriting the first equation:

$$
\begin{aligned}
Vu &= -\frac{\partial v}{\partial t} + \frac{1}{2}\Delta u - \kappa(u^2 + v^2)u \\
&= -\pi u - \frac{n}{2}\pi^2 u - \kappa(u^2 + v^2)u \\
V(\boldsymbol{x}) &= -\pi - \frac{n}{2}\pi^2 - \kappa(u^2 + v^2)
\end{aligned}
$$

And the second equation:

$$
\begin{aligned}
Vv &= \frac{\partial u}{\partial t} + \frac{1}{2}\Delta v - \kappa(u^2 + v^2)v \\
&= -\pi v - \frac{n}{2}\pi^2 v - \kappa(u^2 + v^2)v \\
V(\boldsymbol{x}) &= -\pi - \frac{n}{2}\pi^2 - \kappa(u^2 + v^2)
\end{aligned}
$$

We see that the equations agree.

3 Spatial Discretization

Consider a set of basis function $\mathbf{\Phi}_i : \Omega \to \mathbb{R}^2$, where each $\mathbf{\Phi}_i(\boldsymbol{x}) = \varphi_{b_i}\hat{\mathbf{e}}_{c_i}$, where $\varphi_j : \Omega \to \mathbb{R}$ is a set of basis functions (b_i is the base index of the index i and c_i is the component index of i). We write $\boldsymbol{w} = \begin{bmatrix} u \\ v \end{bmatrix}$ and make the approximation $\boldsymbol{w} = W_j \mathbf{\Phi}_j$ (Einstein summation); furthermore, we approximate $\frac{\partial \boldsymbol{w}}{\partial t} = \dot{W}_j \mathbf{\Phi}_j$. Then, we have that:

$$\begin{aligned}
u &= W_j \varphi_{b_j} \delta_{1,c_j} \\
v &= W_j \varphi_{b_j} \delta_{2,c_j} \\
\frac{\partial u}{\partial t} &= \dot{W}_j \varphi_{b_j} \delta_{1,c_j} \\
\frac{\partial v}{\partial t} &= \dot{W}_j \varphi_{b_j} \delta_{2,c_j}
\end{aligned}$$

Then, we multiply and integrate the system with a basis function $\mathbf{\Phi}_i$:

$$\left\langle \mathbf{\Phi}_i \mid \begin{matrix} \partial_t v - \frac{1}{2}\Delta u + Vu + \kappa(u^2+v^2)u \\ -\partial_t u - \frac{1}{2}\Delta v + Vv + \kappa(u^2+v^2)v \end{matrix} \right\rangle = 0$$

$$\mathrm{i} \left\langle \mathbf{\Phi}_i \mid \begin{matrix} \partial_t v \\ -\partial_t u \end{matrix} \right\rangle - \frac{1}{2} \left\langle \mathbf{\Phi}_i \mid \begin{matrix} \Delta u \\ \Delta v \end{matrix} \right\rangle + \left\langle \mathbf{\Phi}_i \mid \begin{matrix} Vu \\ Vv \end{matrix} \right\rangle + \kappa \left\langle \mathbf{\Phi}_i \mid \begin{matrix} u^3 \\ v^3 \end{matrix} \right\rangle + \kappa \left\langle \mathbf{\Phi}_i \mid \begin{matrix} uv^2 \\ u^2 v \end{matrix} \right\rangle = 0$$

We consider each form separately:

$$\begin{aligned}
\left\langle \mathbf{\Phi}_i \mid \begin{matrix} \partial_t v \\ -\partial_t u \end{matrix} \right\rangle &= \delta_{1,c_i} \langle \varphi_{b_i} \mid \partial_t v \rangle - \delta_{2,c_i} \langle \varphi_{b_i} \mid \partial_t u \rangle \\
&= \delta_{1,c_i} \left\langle \varphi_{b_i} \mid \dot{W}_j \varphi_{b_j} \delta_{2,c_j} \right\rangle - \delta_{2,c_i} \left\langle \varphi_{b_i} \mid \dot{W}_j \varphi_{b_j} \delta_{1,c_j} \right\rangle \\
&= (\delta_{1,c_i}\delta_{2,c_j} - \delta_{2,c_i}\delta_{1,c_j}) \left\langle \varphi_{b_i} \mid \varphi_{b_j} \right\rangle \dot{W}_j
\end{aligned}$$

$$\left\langle \mathbf{\Phi}_i \mid \begin{matrix} \Delta u \\ \Delta v \end{matrix} \right\rangle = \delta_{1,c_i} \langle \varphi_{b_i} \mid \Delta u \rangle + \delta_{2,c_i} \langle \varphi_{b_i} \mid \Delta v \rangle$$

We note that:

$$\begin{aligned}
\langle \varphi_{b_i} \mid \Delta f \rangle &= \int_\Omega \varphi_{b_i} \Delta f \, \mathrm{d}\boldsymbol{x} \\
&= \oint_{\partial\Omega} \varphi_{b_i} \nabla f \cdot \hat{\mathbf{n}} \, \mathrm{d}\boldsymbol{s} - \int_\Omega \nabla \varphi_{b_i} \cdot \nabla f \, \mathrm{d}\boldsymbol{x} \\
&= \langle \varphi_{b_i} \hat{\mathbf{n}} \mid \nabla f \rangle_{\partial\Omega} - \langle \nabla \varphi_{b_i} \mid \nabla f \rangle
\end{aligned}$$

And, because we have Dirichlet boundary conditions, we must have that $\varphi_{b_i}(t, \boldsymbol{x}) = 0$ for all $(t, \boldsymbol{x}) \in (0, T) \times \partial\Omega$. So:

$$\begin{aligned}
\left\langle \mathbf{\Phi}_i \mid \begin{matrix} \Delta u \\ \Delta v \end{matrix} \right\rangle &= -\delta_{1,c_i} \langle \nabla \varphi_{b_i} \mid \nabla u \rangle - \delta_{2,c_i} \langle \nabla \varphi_{b_i} \mid \nabla v \rangle \\
&= -\delta_{1,c_i} \left\langle \nabla \varphi_{b_i} \mid W_j \nabla \varphi_{b_j} \delta_{1,c_j} \right\rangle - \delta_{2,c_i} \left\langle \nabla \varphi_{b_i} \mid W_j \nabla \varphi_{b_j} \delta_{2,c_j} \right\rangle \\
&= -(\delta_{1,c_i}\delta_{1,c_j} + \delta_{2,c_i}\delta_{2,c_j}) \left\langle \nabla \varphi_{b_i} \mid \nabla \varphi_{b_j} \right\rangle W_j
\end{aligned}$$

$$
\begin{aligned}
\left\langle \boldsymbol{\Phi}_i \mid \begin{matrix} Vu \\ Vv \end{matrix} \right\rangle &= \delta_{1,c_i} \langle \varphi_{b_i} \mid Vu \rangle + \delta 2, c_i \langle \varphi_{b_i} \mid Vv \rangle \\
&= \delta_{1,c_i} \left\langle \varphi_{b_i} \mid W_j V \varphi_{b_j} \delta_{1,c_j} \right\rangle + \delta_{2,c_i} \left\langle \varphi_{b_i} \mid W_j V \varphi_{b_j} \delta_{2,c_j} \right\rangle \\
&= (\delta_{1,c_i}\delta_{1,c_j} + \delta_{2,c_i}\delta_{2,c_j}) \left\langle \varphi_{b_i} \mid V \varphi_{b_j} \right\rangle W_j
\end{aligned}
$$

We will not use the fact that $\boldsymbol{w} = W_j \boldsymbol{\Phi}_j$ in considering the nonlinear forms at this time.

So:

$$
\begin{aligned}
0 = &(\delta_{1,c_i}\delta_{2,c_j} - \delta_{2,c_i}\delta_{1,c_j}) \left\langle \varphi_{b_i} \mid \varphi_{b_j} \right\rangle \dot{W}_j \\
&+ \frac{1}{2}(\delta_{1,c_i}\delta_{1,c_j} + \delta_{2,c_i}\delta_{2,c_j}) \left\langle \nabla\varphi_{b_i} \mid \nabla\varphi_{b_j} \right\rangle W_j \\
&+ (\delta_{1,c_i}\delta_{1,c_j} + \delta_{2,c_i}\delta_{2,c_j}) \left\langle \varphi_{b_i} \mid V\varphi_{b_j} \right\rangle W_j \\
&+ \kappa\delta_{1,c_i} \left\langle \varphi_{b_i} \mid u^3 + uv^2 \right\rangle \\
&+ \kappa\delta_{2,c_i} \left\langle \varphi_{b_i} \mid v^3 + u^2 v \right\rangle
\end{aligned}
$$

If we define:

$$
\begin{aligned}
M_{ij} &= (\delta_{1,c_i}\delta_{2,c_j} - \delta_{2,c_i}\delta_{1,c_j}) \left\langle \varphi_{b_i} \mid \varphi_{b_j} \right\rangle \\
A_{ij} &= \frac{1}{2}(\delta_{1,c_i}\delta_{1,c_j} + \delta_{2,c_i}\delta_{2,c_j}) \left\langle \nabla\varphi_{b_i} \mid \nabla\varphi_{b_j} \right\rangle \\
B_{ij} &= (\delta_{1,c_i}\delta_{1,c_j} + \delta_{2,c_i}\delta_{2,c_j}) \left\langle \varphi_{b_i} \mid V\varphi_{b_j} \right\rangle \\
C_i &= \kappa\delta_{1,c_i} \left\langle \varphi_{b_i} \mid u^3 + uv^2 \right\rangle + \kappa\delta_{2,c_i} \left\langle \varphi_{b_i} \mid v^3 + u^2 v \right\rangle
\end{aligned}
$$

We rewrite the above equation as:

$$
\mathbf{0} = \boldsymbol{M}\dot{\boldsymbol{W}} + (\boldsymbol{A} + \boldsymbol{B})\boldsymbol{W} + \boldsymbol{C}
$$

4 Time Stepping

In order to solve the monolithic system using an implicit Runge-Kutta method, we rewrite the equation from the previous section:

$$\begin{aligned}
\boldsymbol{M}\dot{\boldsymbol{W}} &= -(\boldsymbol{A}+\boldsymbol{B})\boldsymbol{W} - \boldsymbol{C} \\
\dot{\boldsymbol{W}} &= -\boldsymbol{M}^{-1}((\boldsymbol{A}+\boldsymbol{B})\boldsymbol{W} + \boldsymbol{C}) \\
&= \boldsymbol{F}(\boldsymbol{W})
\end{aligned}$$

We must compute the action of $(\mathbf{I} - \tau\mathbf{J}[\boldsymbol{F}])^{-1}$ on a vector. We have that:

$$\begin{aligned}
\mathbf{J}[\boldsymbol{F}] &= \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{W}} \\
&= -\frac{\partial}{\partial \boldsymbol{W}}(\boldsymbol{M}^{-1}((\boldsymbol{A}+\boldsymbol{B})\boldsymbol{W} + \boldsymbol{C})) \\
&= -\boldsymbol{M}^{-1}\frac{\partial}{\partial \boldsymbol{W}}((\boldsymbol{A}+\boldsymbol{B})\boldsymbol{W} + \boldsymbol{C}) \\
&= -\boldsymbol{M}^{-1}((\boldsymbol{A}+\boldsymbol{B}) + \mathbf{J}[\boldsymbol{C}]) \\
\boldsymbol{M}\mathbf{J}[\boldsymbol{F}] &= -\boldsymbol{A} - \boldsymbol{B} - \mathbf{J}[\boldsymbol{C}]
\end{aligned}$$

The matrix $\mathbf{J}[\boldsymbol{C}]$ is less easy to compute, but can be computed by automatic differentiation. Then:

$$\begin{aligned}
(\mathbf{I} - \tau\mathbf{J}[\boldsymbol{F}])\boldsymbol{x} &= \boldsymbol{b} \\
\boldsymbol{M}(\mathbf{I} - \tau\mathbf{J}[\boldsymbol{F}])\boldsymbol{x} &= \boldsymbol{M}\boldsymbol{b} \\
(\boldsymbol{M} + \tau(\boldsymbol{A}+\boldsymbol{B}+\mathbf{J}[\boldsymbol{C}]))\boldsymbol{x} &= \boldsymbol{M}\boldsymbol{b}
\end{aligned}$$

Solving for $\boldsymbol{x}$ in the above equation is equivalent to multiplication by $(\mathbf{I} - \tau\mathbf{J}[\boldsymbol{F}])^{-1}$. This action is used in implicit Runge-Kutta time stepping.