1 Introduction

This document is relevant to the targets:

- `monolithic`
- `monolithic_arkode`
- `monolithic_hs`

See the "Version History" section for more information. The section "Toy Problem" is unimplemented.

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:

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

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

We note that:

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

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:

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

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

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:

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

4 Time Stepping

In order to solve the monolithic system using Crank-Nicolson time stepping, we write:

$$\begin{aligned}
\mathbf{0} &= \frac{1}{h}\boldsymbol{M}(\boldsymbol{W}_{k+1} - \boldsymbol{W}_k) + \frac{1}{2}(\boldsymbol{A}+\boldsymbol{B})(\boldsymbol{W}_{k+1} + \boldsymbol{W}_k) + \frac{1}{2}(\boldsymbol{C}_{k+1} + \boldsymbol{C}_k) \\
\mathbf{0} &= \boldsymbol{M}(\boldsymbol{W}_{k+1} - \boldsymbol{W}_k) + \frac{h}{2}(\boldsymbol{A}+\boldsymbol{B})(\boldsymbol{W}_{k+1} + \boldsymbol{W}_k) + \frac{h}{2}(\boldsymbol{C}_{k+1} + \boldsymbol{C}_k)
\end{aligned}$$

Where h is the chosen time step. So, define:

$$\begin{aligned}
\boldsymbol{R}_k(\boldsymbol{W}) &= \boldsymbol{M}(\boldsymbol{W} - \boldsymbol{W}_k) + \frac{h}{2}(\boldsymbol{A}+\boldsymbol{B})(\boldsymbol{W} + \boldsymbol{W}_k) + \frac{h}{2}(\boldsymbol{C} + \boldsymbol{C}_k) \\
&= (\boldsymbol{M} + \frac{h}{2}(\boldsymbol{A}+\boldsymbol{B}))\boldsymbol{W} + \frac{h}{2}\boldsymbol{C} + (-\boldsymbol{M} + \frac{h}{2}(\boldsymbol{A}+\boldsymbol{B}))\boldsymbol{W}_k + \frac{h}{2}\boldsymbol{C}_k
\end{aligned}$$

Recall that $\boldsymbol{C}$ can be defined by $\boldsymbol{W}$. To step from time step k to $k+1$, we must solve $\boldsymbol{R}_k(\boldsymbol{W}) = \mathbf{0}$; we do so using Newton iteration, i.e., we repeatedly solve:

$$\begin{aligned}
\mathbf{J}_{\boldsymbol{W}_k^{(\ell)}}[\boldsymbol{R}_k]\Delta\boldsymbol{W}_k^{(\ell)} &= -\boldsymbol{R}_k(\boldsymbol{W}_k^{(\ell)}) \\
\boldsymbol{W}_k^{(\ell+1)} &= \boldsymbol{W}_k^{(\ell)} + \alpha_k \Delta\boldsymbol{W}_k^{(\ell)}
\end{aligned}$$

Where $\mathbf{J}_{\boldsymbol{W}_k^{(\ell)}}[\boldsymbol{R}_k]$ is the Jacobian matrix of $\boldsymbol{R}_k$ evaluated at $\boldsymbol{W}_k^{(\ell)}$ and α_k is a step size chosen by the Newton solver. Once the residual norm $\|\boldsymbol{W}_k^{(\ell)}\|$ is sufficiently small, we take $\boldsymbol{W}_{k+1} = \boldsymbol{W}_k^{(\ell)}$.

So, we must compute $\mathbf{J}_{\boldsymbol{W}_k^{(\ell)}}[\boldsymbol{R}_k]$:

$$\begin{aligned}
\mathbf{J}[\boldsymbol{R}_k] &= \frac{\partial \boldsymbol{R}_k}{\partial \boldsymbol{W}} \\
&= \boldsymbol{M} + \frac{h}{2}(\boldsymbol{A}+\boldsymbol{B}) + \frac{h}{2}\frac{\partial \boldsymbol{C}}{\partial \boldsymbol{W}} \\
&= \boldsymbol{M} + \frac{h}{2}(\boldsymbol{A}+\boldsymbol{B}) + \frac{h}{2}\mathbf{J}[\boldsymbol{C}]
\end{aligned}$$

The Jacobian of $\boldsymbol{C}$ is more difficult to write, but $\mathbf{J}_{\boldsymbol{W}_k^{(\ell)}}[\boldsymbol{C}]$ can be computed using automatic differentiation.

5 Version History

The target `monolithic` implements the above problem without matrices and using only automatic differentiation. `monolithic_arkode` is similar but uses the SUNDIALS ARKODE solver; the detail of the solution is extremely low. `monolithic_hs` uses the method described above, which avoids unnecessary differentiation, although the results are not identical to those produced by `monolithic`.