Meshfree integrators<br>Marco Caliari, Alexander Ostermann, Stefan Rainer

## 1. Introduction

We consider the time-dependent partial differential equation

$$
\begin{equation*}
\frac{\partial}{\partial t} u(t, \xi)=F\left(t, \xi, u(t, \xi), \frac{\partial}{\partial \xi} u(t, \xi), \ldots\right), \quad t \in[0, T], \quad \xi \in \Omega \subset \mathbb{R}^{d} \tag{1}
\end{equation*}
$$

subject to appropriate initial and boundary conditions. We assume that the essential support of the solution, that is the closure of the set of points where the magnitude of the solution is greater than some given threshold, is small with respect to the domain of interest, and varying in time.

For the numerical solution of (1), we propose a meshfree integrator based on stable and robust interpolation by compactly supported radial basis functions for the spatial approximation and exponential integrators for the time evolution. Our meshfree integrator controls the error both in space and time.

## 2. Meshfree integrators

In this section we briefly describe how we compute the numerical approximation $u_{n}(\xi) \approx u\left(t_{n}, \xi\right)$ for discrete times $0=t_{0}<t_{1}<\ldots<t_{N}=T$. For a detailed description of the method, we refer to [2]. Given an approximation $u_{n-1}(\xi)$ at time $t_{n-1}$, we interpolate it by compactly supported radial basis functions

$$
u_{n}(\xi) \approx s(\xi)=\sum_{\eta \in H} \lambda_{\eta} \phi(\|\xi-\eta\|)
$$

using a set of interpolation points $H=\left\{\eta_{1}, \ldots, \eta_{m}\right\}$. The coefficients $\lambda_{\eta}$ are determined from the interpolation conditions $s\left(\eta_{i}\right)=u_{n-1}\left(\eta_{i}\right), i=1, \ldots, m$. In order to control the spatial interpolation error, we update the set of interpolation points using a residual subsampling method. For this purpose, we measure the difference between $u_{n-1}$ and its interpolant at a different set of check points. We update the set of interpolation points (by a coarsening and a refinement procedure) until the error at all check points lies between two given thresholds $\theta_{\mathrm{c}}<\theta_{\mathrm{r}}$.

Approximating the right-hand side in (1) we obtain a system of stiff ordinary differential equations

$$
w^{\prime}(t)=G_{n}(t, w(t)), \quad t \in\left[t_{n-1}, t_{n}\right]
$$

where the vector $w\left(t_{n-1}\right)$ contains the values of $u_{n-1}(\xi)$ at the interpolation and check points. This system is solved with an exponential integrator. For a review of such integrators, we refer to [6]. The required actions of matrix functions are computed with the Real Leja Points Method (see, e.g., [5, 2]).

The numerical solution $u_{n}(\xi)$ is finally constructed from the numerical approximation to $w\left(t_{n}\right)$. In order to control the error in time we use an embedded method. The error in space is again controlled by a residual subsampling method. Unless both errors are sufficiently small, we repeat the time step by taking a smaller step size and/or a different set of interpolation points.

## 3. Numerical example

We consider the solution of the nonlinear Schrödinger equation

$$
\left\{\begin{align*}
\mathrm{i} \varepsilon \partial_{t} \psi & =-\frac{\varepsilon^{2}}{2} \Delta \psi+V(x, y) \psi-|\psi|^{2 p} \psi, \quad(x, y) \in \mathbb{R}^{2}, t>0  \tag{2}\\
\psi(0, x, y) & =\psi_{0}(x, y)
\end{align*}\right.
$$

where $0<p<1$. As initial value we take a two-bump solution

$$
\psi_{0}(x, y)=\sum_{j=1}^{2} r\left(\frac{x-\bar{x}_{j}}{\varepsilon}, \frac{y-\bar{y}_{j}}{\varepsilon}\right)
$$

where $\bar{x}_{j}, \bar{y}_{j}$ are given offset centres and $r(x, y) \mathrm{e}^{-\mathrm{i} \lambda t}$ is the ground state solution (see, e.g., [3]) of the associated nonlinear potential-free Schrödinger equation

$$
\mathrm{i} \partial_{t} \phi=-\frac{1}{2} \Delta \phi-|\phi|^{2 p} \phi, \quad\|\phi\|_{L^{2}}^{2}=m
$$

that is the solution $\phi(t, x, y)=r(x, y) \mathrm{e}^{-\mathrm{i} \lambda t}$ minimising the energy

$$
E(\phi)=E(r)=\frac{1}{2} \int_{\mathbb{R}^{2}}|\nabla r|^{2} \mathrm{~d} x \mathrm{~d} y-\frac{1}{p+1} \int_{\mathbb{R}^{2}}|r|^{2 p+2} \mathrm{~d} x \mathrm{~d} y .
$$

From Newton's laws

$$
\left\{\begin{align*}
{\left[\ddot{x}_{j}(t), \ddot{y}_{j}(t)\right] } & =-\nabla V(x(t), y(t)),  \tag{3}\\
{\left[x_{j}(0), y_{j}(0)\right] } & =\left[\bar{x}_{j}, \bar{y}_{j}\right], \quad\left[\dot{x}_{j}(0), \dot{y}_{j}(0)\right]=[0,0] \quad \text { for } j=1,2
\end{align*}\right.
$$

one infers (see [4]) that the solution of (2) behaves like

$$
\sum_{j=1}^{2} r\left(\frac{x-x_{j}(t)}{\varepsilon}, \frac{y-y_{j}(t)}{\varepsilon}\right) \exp \left(\frac{\mathrm{i}}{\varepsilon}\left(x \dot{x}_{j}(t)+y \dot{y}_{j}(t)+\theta_{j}^{\varepsilon}(t)\right)\right)
$$

where $\theta_{j}^{\varepsilon}: \mathbb{R}^{+} \rightarrow[0,2 \pi), j=1,2$ are suitable shifts, up to an error depending on $\varepsilon$. This dynamical behaviour, in which the shape of $\psi(t, x, y)$ remains close to that of the initial value $\psi_{0}(x, y)$, is typically known as soliton dynamics.

In order to solve (2), we apply the fourth-order splitting method $\operatorname{SRKN}_{6}^{b}$ by Blanes and Moan [1]. The first part of the equation, with the Laplacian, is approximated in space using Wendland's compactly supported radial basis function $\phi_{3,2}$ (see [7]) and exactly integrated in time using an exponential integrator. The second part, with the potential and the nonlinear term, has an analytic solution.

In Figure 1 we show the behaviour of the solution of (2) for

$$
\varepsilon=0.01, \quad p=0.2, \quad V(x, y)=\frac{3}{2} x^{2}+y^{2}
$$

with $\bar{x}_{1}=-3, \bar{x}_{2}=3, \bar{y}_{1}=\bar{y}_{2}=-3$ at different times $t$. In this case, the solutions of (3) are analytically known (they lie on Lissajous curves). We observe that the shape of the two bumps is well preserved during time integration, their centres of mass follow the Lissajous curves. Moreover, the location of the interpolation points is always well spread around the essential support of the solution.


Figure 1. Contour levels of the solution (left) and location of interpolation points (right) at different times $t$.

## References

[1] S. Blanes and P. C. Moan, Practical symplectic partitioned Runge-Kutta and Runge-KuttaNyström methods, J. Comput. Appl. Math. 142 (2002), 313-330.
[2] M. Caliari, A. Ostermann, and S. Rainer, Meshfree exponential integrators, submitted (2010).
[3] M. Caliari, A. Ostermann, S. Rainer, and M. Thalhammer, A minimisation approach for computing the ground state of Gross-Pitaevskii systems, J. Comput. Phys. 228 (2009), 349-360.
[4] M. Caliari and M. Squassina, Numerical computation of soliton dynamics for NLS equations in a driving potential, Electron. J. Diff. Eqns. 89 (2010), 1-12.
[5] M. Caliari, M. Vianello, and L. Bergamaschi, Interpolating discrete advection-diffusion propagators at Leja sequences, J. Comput. Appl. Math. 172 (2004), 79-99.
[6] M. Hochbruck and A. Ostermann, Exponential integrators, Acta Numerica 19 (2010), 209286.
[7] H. Wendland, Piecewise polynomial, positive definite and compactly supported radial functions of minimal degree, Adv. Comput. Math. 4 (1995), 389-396.

