Lecture 3: Time-integration of magnetic variational wave packets and more

Caroline Lasser (TUM)

joint work with

Marlis Hochbruck, Malik Scheifinger (Karlsruhe), Kurt Busch (Berlin)

Simen Kvaal, Thomas Pedersen (Oslo), Ludwik Adamowicz (Tucson)

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Short review on lectures 1 & 2

Lecture 1: Variational approximation

Choose a manifold $\mathcal{M} \subset \mathcal{H}$.

Determine $u(t) \approx \psi(t)$, $u(t) \in \mathcal{M}$ as follows:

1. $\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$

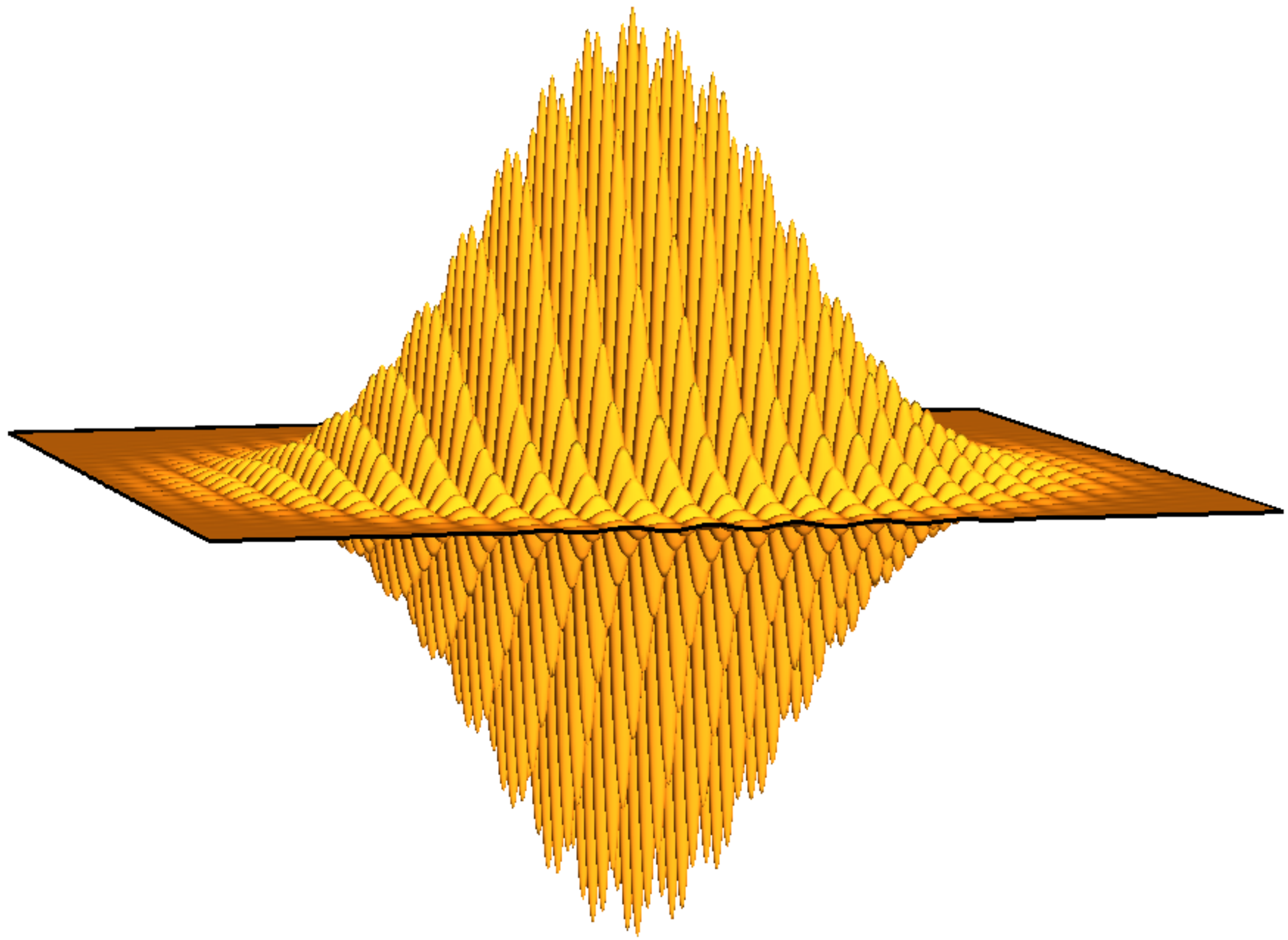
2. $\|i\partial_t u(t) - H(t)u(t)\|_{\mathcal{H}} = \min_{\partial_t u(t)}!$

Parametric approximation chooses

$$\mathcal{M} = \left\{ \Phi(q) : q \in \mathbb{C}^N \right\}$$

for $\Phi : \mathbb{C}^N \to \mathcal{H}$ with $\Phi'(q)$ of constant rank for all q.

$d = 2$



Lecture 2: Variational magnetic Gaussians

$H(t) = \frac{1}{2}(-i\varepsilon\nabla_x - A(t,x))^2 + \varphi(t,x)$

$u(t,x) = \exp\Big(\frac{i}{\varepsilon}\Big(\frac{1}{2}(x-q_t)\cdot P_t Q_t^{-1}(x-q_t) + p_t\cdot(x-q_t) + \zeta_t\Big)\Big)$

Magnetic momenta: $v_t := p_t - \langle A\rangle$, $\Upsilon_t := P_t - \langle A'\rangle Q_t$

Variational equations of motion:

$$\dot q_t = v_t, \quad \dot v_t = v_t + \langle\nabla\times A\rangle + E^\varepsilon(q_t, v_t, Q_t, \Upsilon_t),$$
$$\dot Q_t = \Upsilon_t, \quad \dot\Upsilon_t = \Upsilon_t \times \langle\nabla\times A\rangle + \mathcal{E}^\varepsilon(q_t, v_t, Q_t, \Upsilon_t)Q_t.$$

Norm and **observable** accuracy: $\mathcal{O}(\sqrt{\varepsilon})$ and $\mathcal{O}(\varepsilon^2)$.

Time-integration

Let $t_n = n\tau$ for $n \in \mathbb{N}$ and step-size $\tau > 0$.

Use a time-stepping scheme to compute

$$(q^n, Q^n, p^n, P^n, \zeta^n) \approx (q(t_n), Q(t_n), p(t_n), P(t_n), \zeta(t_n))$$

and then $u^n \approx u(t_n)$.

For a scheme of order $p \geq 1$, we have for any $T > 0$ a constant $c > 0$ such that

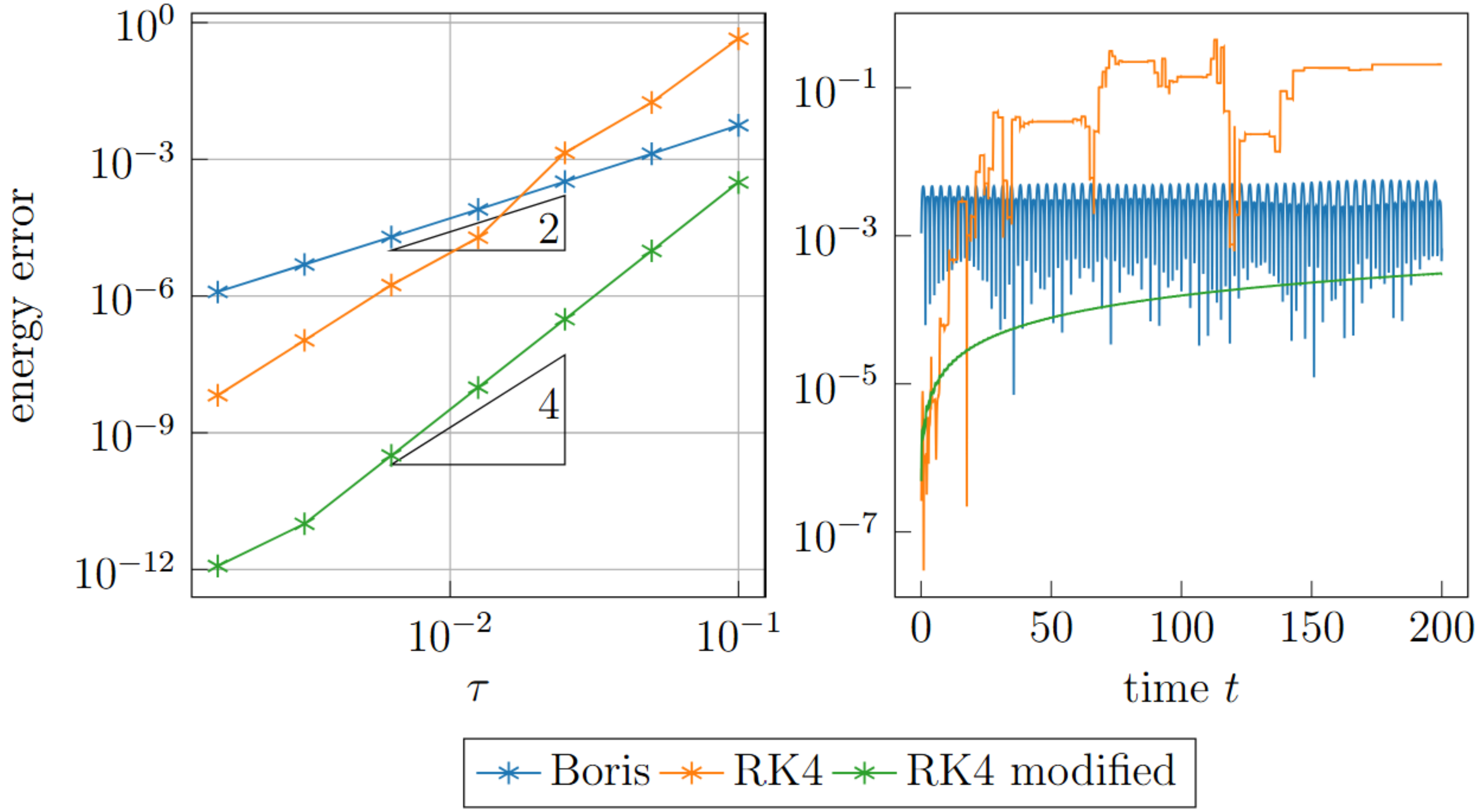
$$\|u^n - u(t_n)\| \leq c \, \frac{\tau^p}{\varepsilon}$$

for all $t_n \leq T$.

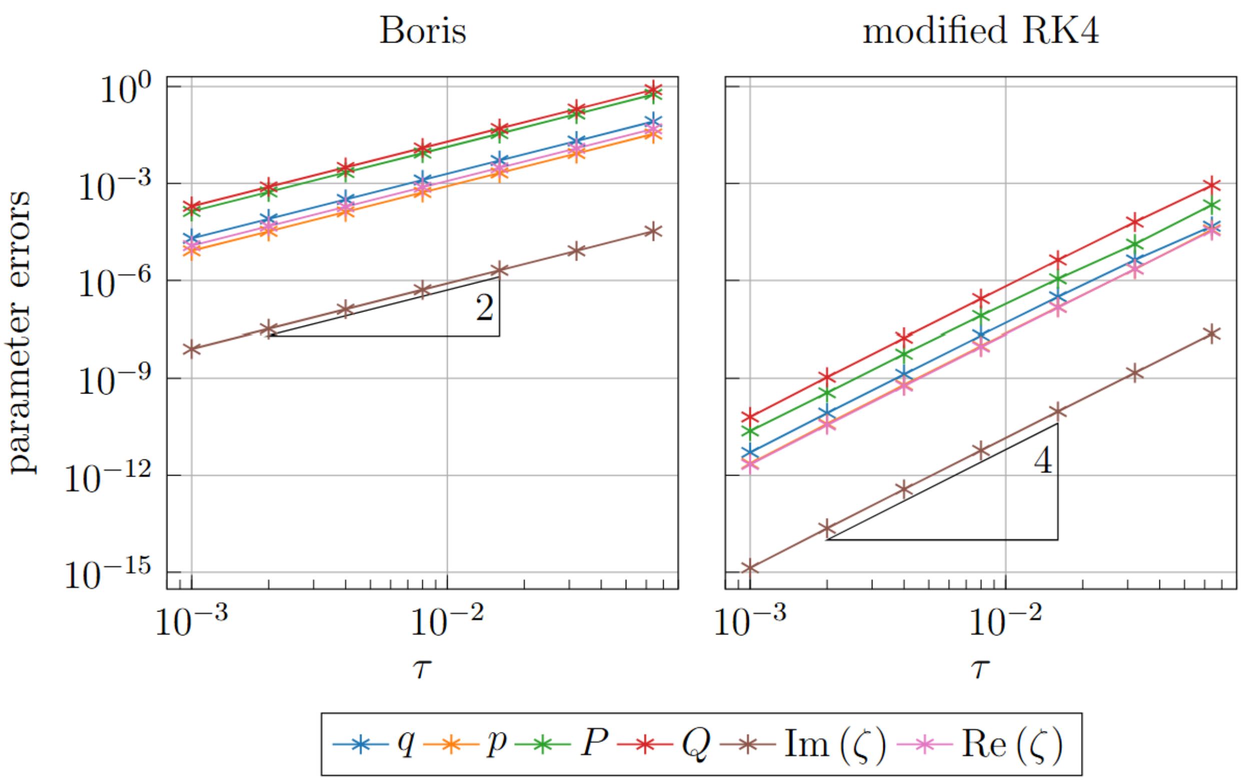
$$H = \frac{1}{2}(-i\varepsilon\nabla_x - A(t,x))^2 + \varphi(x)$$

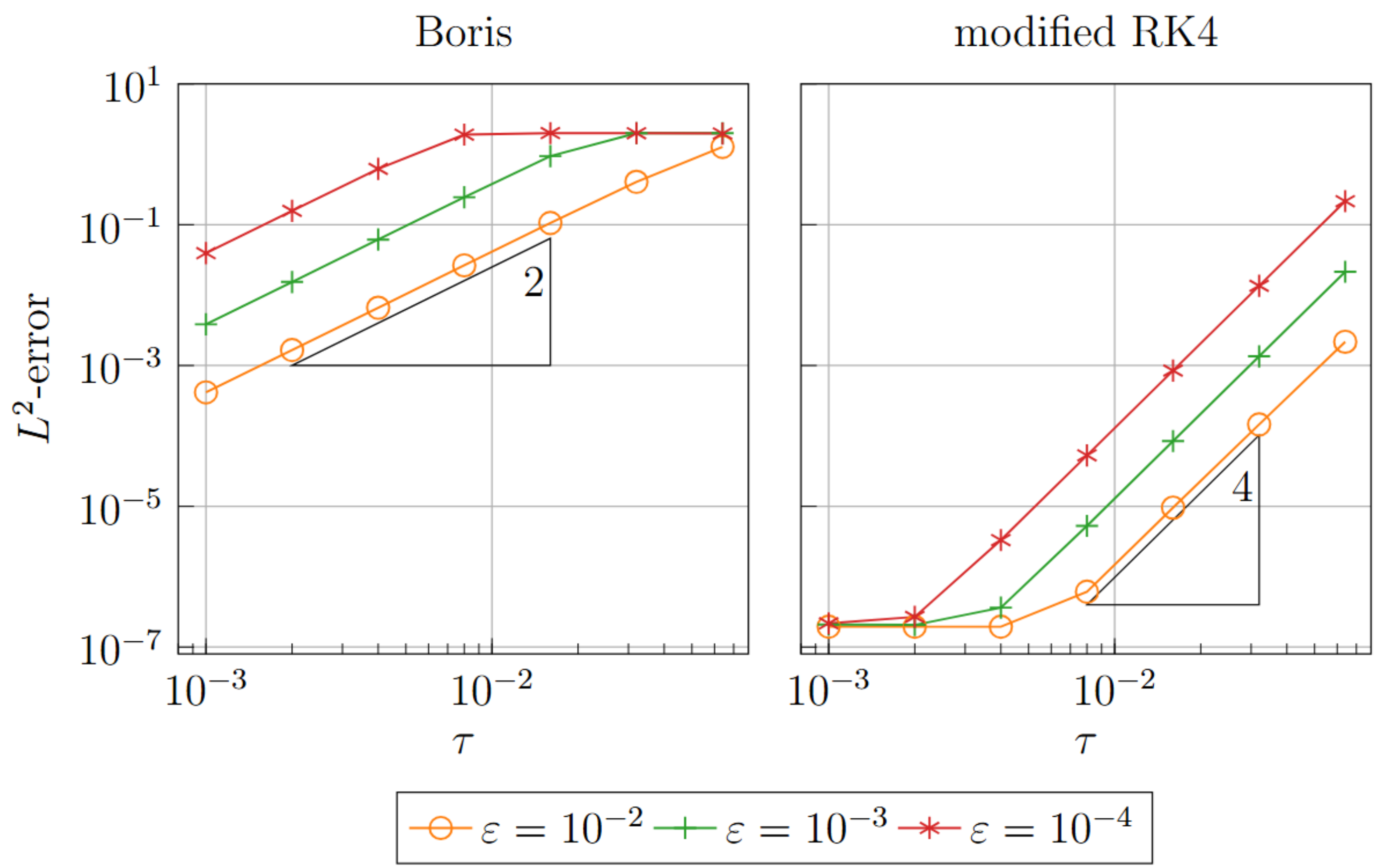
with

$$\begin{aligned} A(t,x) &= \begin{pmatrix} \sin(x_1 + x_2 + \alpha t) \\ -\sin(x_1 + x_2 + \alpha t) \end{pmatrix}, \ \alpha \in \{0,1\} \\ \varphi(x) &= \sin(x_1 + x_2), \\ \varepsilon &= 10^{-3}, \\ T &\in \{8, 200\}. \end{aligned}$$



energy error
10^0
10^{-3}
10^{-6}
10^{-9}
10^{-12}
2
4
10^{-2}
10^{-1}
τ
10^{-1}
10^{-3}
10^{-5}
10^{-7}
0
50
100
150
200
time t
Boris
RK4
RK4 modified


Boris
modified RK4
parameter errors
10^{0}
10^{-3}
10^{-6}
10^{-9}
10^{-12}
10^{-15}
10^{-3}
10^{-2}
τ
2
4
q p P Q $\mathrm{Im}(\zeta)$ $\mathrm{Re}(\zeta)$



Boris
modified RK4
10^{1}
10^{-1}
10^{-3}
10^{-5}
10^{-7}
L^2-error
2
4
10^{-3}
10^{-2}
τ
$\varepsilon = 10^{-2}$
$\varepsilon = 10^{-3}$
$\varepsilon = 10^{-4}$

The convenient modification

$$u(t,x) = \exp\Big(\tfrac{i}{\varepsilon}\Big(\tfrac{1}{2}(x-q_t)\cdot P_t Q_t^{-1}(x-q_t) + p_t\cdot(x-q_t) + \zeta_t\Big)\Big)$$

$t \mapsto \mathrm{Im}(\zeta_t)$ is a continuous normalisation.

$$\mathrm{Im}(\zeta_t) = \mathrm{Im}(\zeta_0) + \tfrac{\varepsilon}{2}\left(\ln|\det Q_t| - \ln|\det Q_0|\right)$$

$$\mathrm{Im}(\zeta^{n+1}) = \mathrm{Im}(\zeta^n) + \tfrac{\varepsilon}{2}\Big(\ln|\det Q^{n+1}| - \ln|\det Q^n|\Big)$$

Runge–Kutta on one slide

$\dot{y} = f(y)$, $y(0) = y_0$

$y_{n+1} = y_n + \tau \sum_{j=1}^{s} b_j \xi_j$ for $n \geq 0$

$\xi_j = f(y_n + \tau \sum_{k=1}^{s} a_{jk} \xi_k)$ for $j = 1, \ldots, s$ (s stages)

$b \in \mathbb{R}^s$, $A \in \mathbb{R}^{s \times s}$

If A is lower triangular, then only f evaluations are needed.

Otherwise, one needs nonlinear solves.

Boris on one slide

$\dot{q} = v$, $\dot{v} = v \times B + E$ with $B = \nabla_x \times A$

$q^n \approx q(t_n)$, $v^n \approx v(t_n - \frac{1}{2}\tau)$

$$\frac{1}{\tau}\left(q^{n+1} - q^n\right) = v^{n+1}$$

$$\frac{1}{\tau}\left(v^{n+1} - v^n\right) = \frac{1}{2}\left(v^n + v^{n+1}\right) \times B(t_n) + E(t_n)$$

$v \times B =: \widehat{B} v$ with $\widehat{B} = -\widehat{B}^\top$ allows to introduce a Cayley transform

Conventional multi-Gaussians

HD molecule

4 particles: 2 electrons, 1 proton, 1 deuteron

The center of mass

$$R = \frac{1}{M_1 + \ldots + M_4} \sum_{n=1}^{4} M_n r_n$$

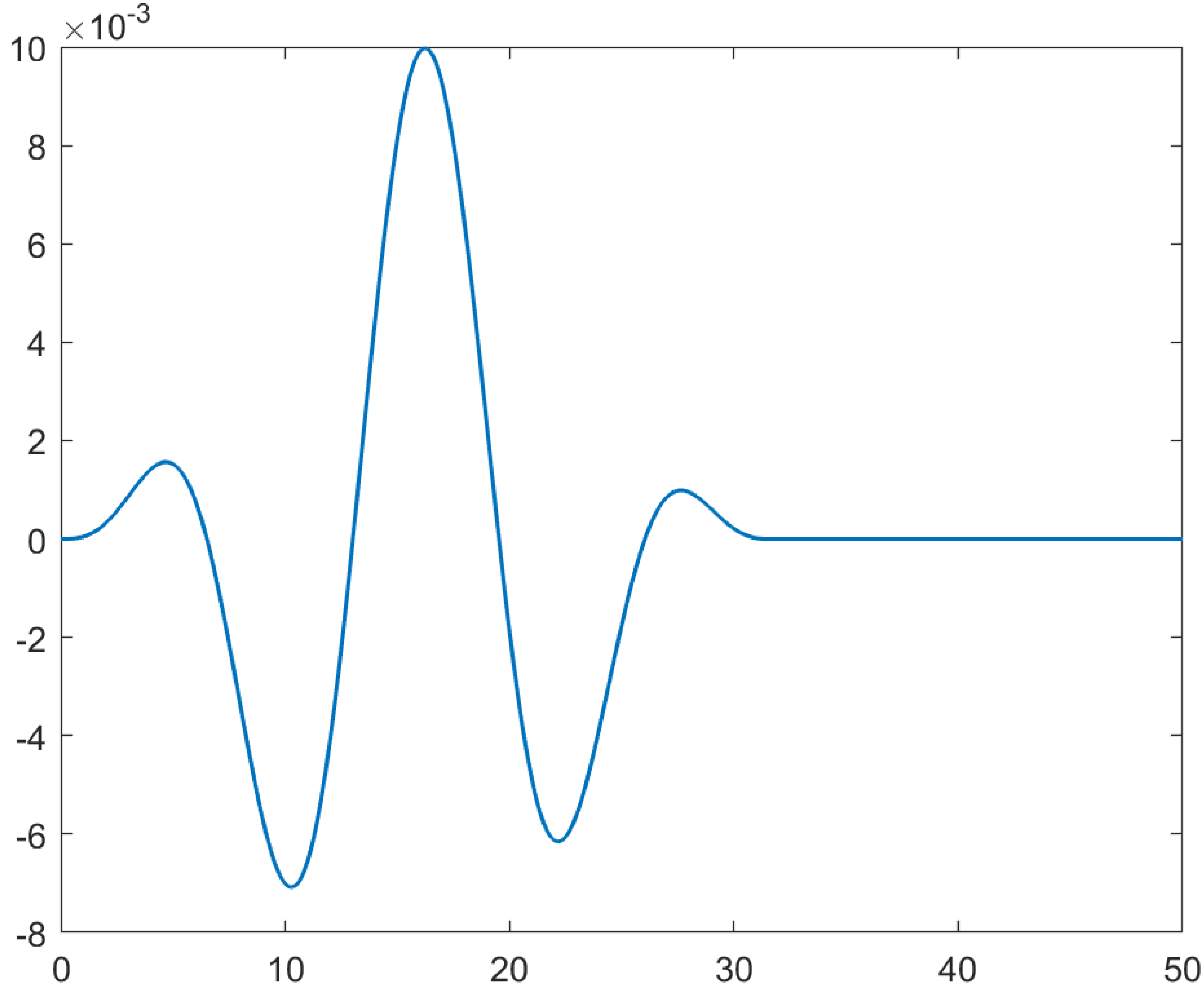
can be separated.

▷ 3 pseudo-particles: 2 pseudo-electrons, 1 pseudo-proton

$$
\begin{aligned}
H \;=\; & \sum_{n=1}^{3} -\frac{1}{2m_n}\left(\partial_{x_n}^2 + \partial_{y_n}^2 + \partial_{z_n}^2\right) + \frac{q_0 q_n}{|r_n|} \\
& + \sum_{n=1}^{2} \sum_{m=n+1}^{3} \frac{q_m q_n}{|r_m - r_n|} \\
& + \sum_{n=1}^{2} \sum_{m=n+1}^{3} \frac{1}{M_D}\left(\partial_{x_n}\partial_{x_m} + \partial_{y_n}\partial_{y_m} + \partial_{z_n}\partial_{z_m}\right)
\end{aligned}
$$

Charge: $q_n = \pm 1$

Mass: $m_n \in \{0.9997, 1224\}$, $M_D = 3670$



×10^-3
10
8
6
4
2
0
-2
-4
-6
-8
0
10
20
30
40
50

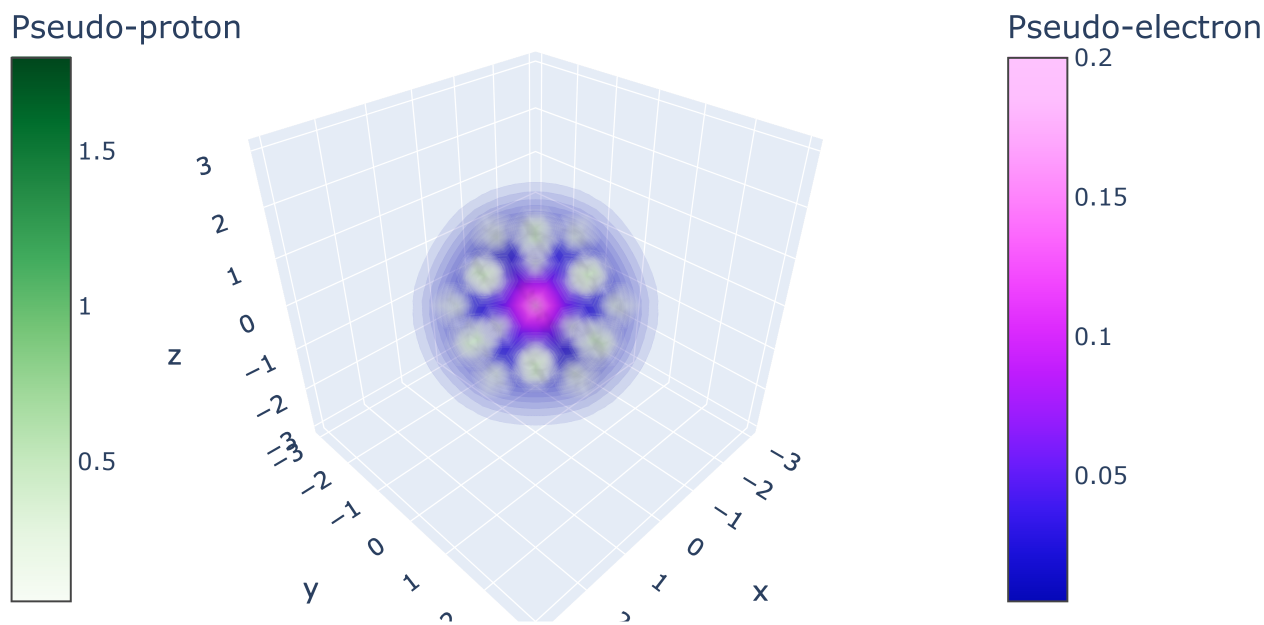
Discretisation

$$u(t,x) = \sum_{n=1}^{N} c_n(t)\,\mathrm{exp}(-(x-q_n)^\top A_n(x-q_n))$$

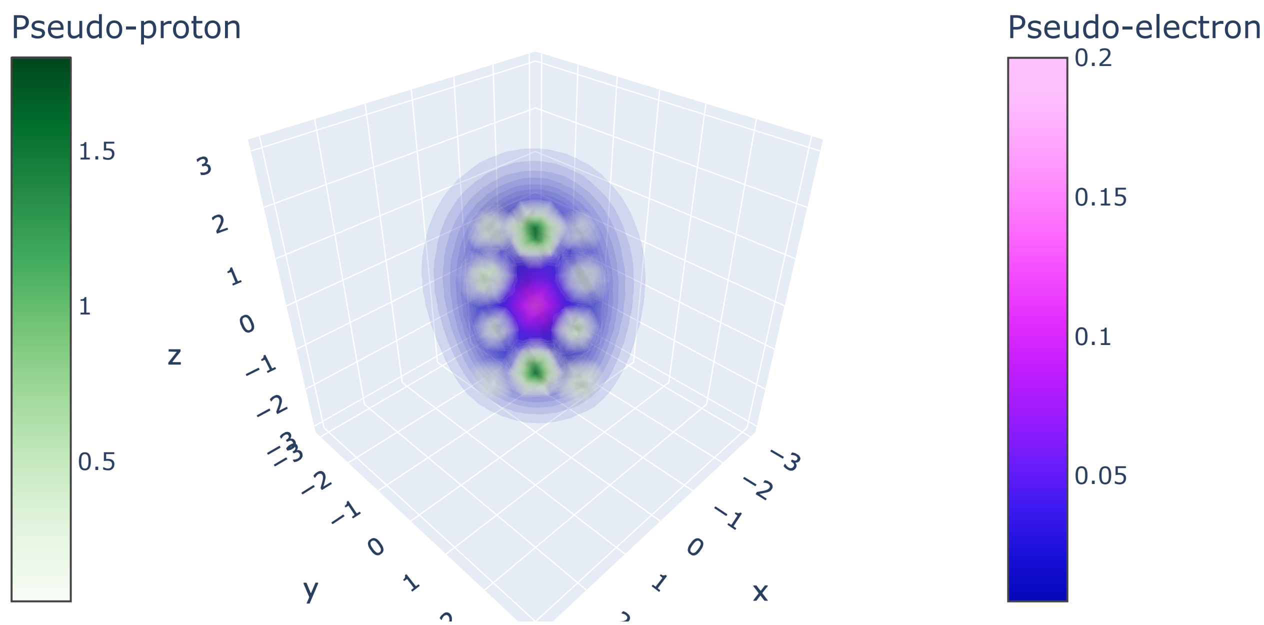
$c_n(t) \in \mathbb{C}$, $q_n \in \mathbb{R}^9$, $N = 1000$

$A_n = A_n^\top \in \mathbb{R}^{9\times 9}$ with $\mathrm{Re}(A_n) > 0$ and anti-symmetrised for the 2 pseudo-electrons

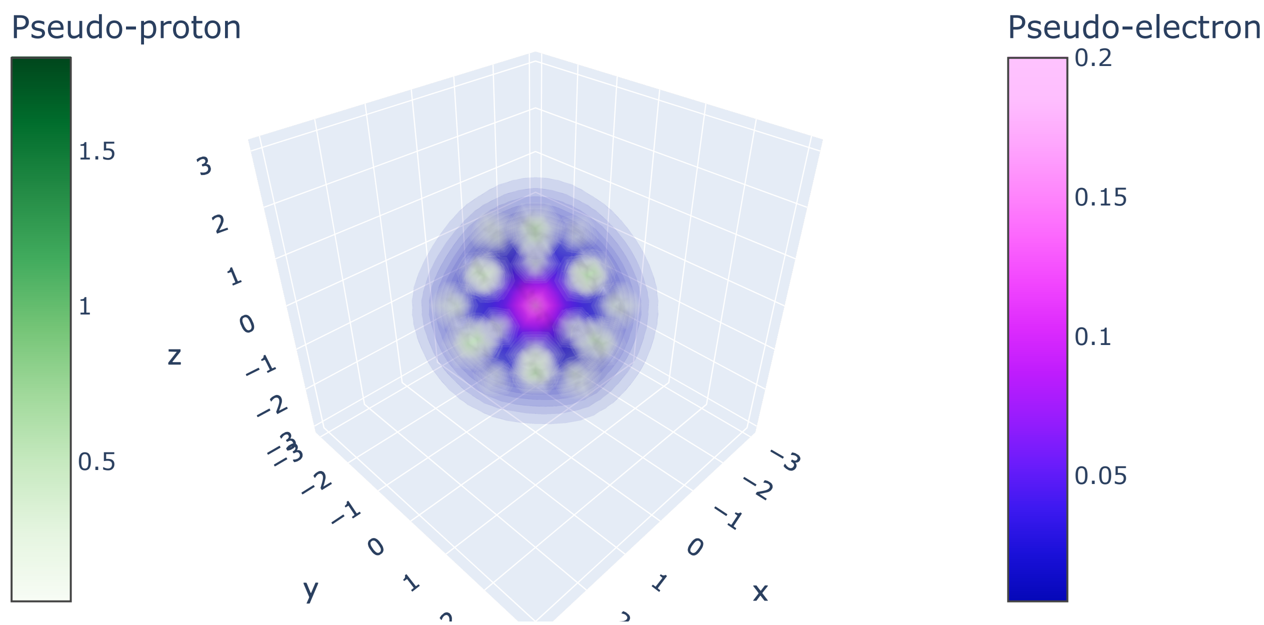
in time: implicit Runge–Kutta method of order six



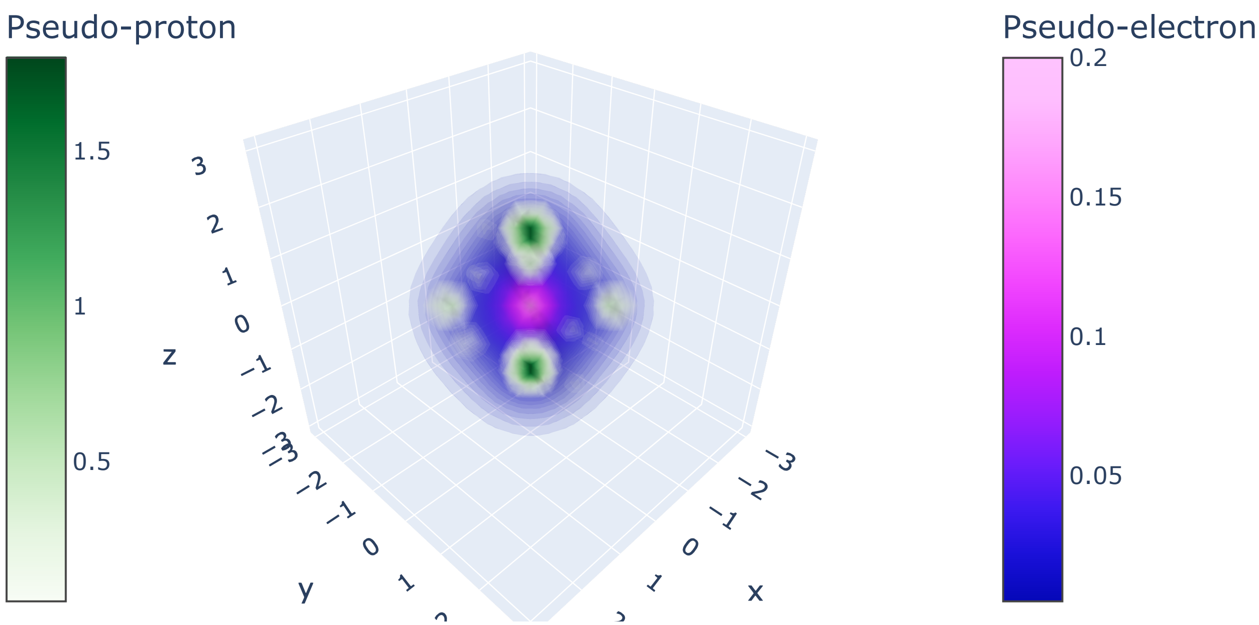
$t = 0\text{fs}$



$t = 16$fs



$t = 470$fs



$t = 530\text{fs}$

Thank you.