AN ENERGY PRESERVING METHOD FOR THE SCHRÖDINGER-POISSON SYSTEM

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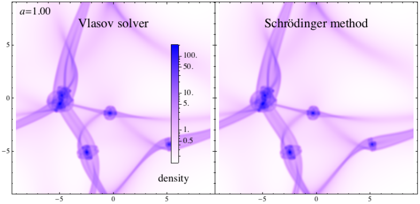
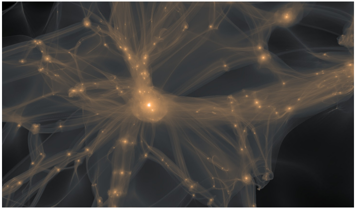
Why Schrödinger - Poisson system (SPS)?

Physical Applications

- Semiconductor modelling; Plasma physics
- Cosmology; in particular galaxy formation



Kopp, Vattis & Scordis, 2017



From the page of Dr. R. Kaehler

2d & 3d simulations for galaxy formation

Challenges

- Interesting physical quantities (e.g., position density) develop *sharply localised* features
- Accurate numerical approximations with uniform meshes would require *extremely fine* spatial & temporal mesh sizes
- Uniform meshes in 2d & 3d: hardly practical

The continuous problem

$$\begin{cases} \partial_t u - \mathrm{i}\dfrac{\varepsilon}{2\alpha^2}\Delta u + \mathrm{i}\dfrac{\beta}{\varepsilon\alpha} v u = 0, \quad \Delta v = |u|^2 & \text{in } \Omega \times [0, T], \\ u = 0, \quad v = 0 & \text{on } \partial\Omega \times [0, T], \\ u(\cdot, 0) = u_0 & \text{in } \Omega, \end{cases}$$

- Ω: convex polygonal domain in $\mathbb{R}^d$, $d = 1, 2, 3$
- $u_0 : \Omega \to \mathbb{C}$ given initial value; $u_0 \in H_0^1(\Omega) \cap H^2(\Omega)$
- $\alpha, \varepsilon > 0$
- $\beta \in \mathbb{R}$ ($\beta > 0 \Rightarrow$ focusing (or attractive), $\beta < 0 \Rightarrow$ defocusing (or repulsive))

❍ Existence of a unique smooth solution (u, v) (Castella, 1997; Bourgain, 1999)

- Often in the *PDE literature*: $v = |u|^2 * K$, K appropriate Green's function

Time discretisation: A relaxation scheme

1. Rewrite SPS as the following system:

$$\begin{cases} \partial_t u - \mathrm{i}\dfrac{\varepsilon}{2\alpha^2}\Delta u + \mathrm{i}\dfrac{\beta}{\varepsilon\alpha} v u = 0 & \text{in } \Omega \times (0, T] \\ \Delta v = \phi, \quad \phi = |u|^2 & \text{in } \Omega \times (0, T], \end{cases}$$

❍ Notation:

- $0 =: t_0 < t_1 < \cdots < t_N := T$ a partition of $[0, T]$, $I_n := (t_n, t_{n+1}]$,

$$k_n := t_{n+1} - t_n \text{ the variable time steps}, \; k := \max_{0 \le n \le N-1} k_n$$

- $\bar{\partial} U^n := \dfrac{U^{n+1} - U^n}{k_n}$, $U^{n+\frac{1}{2}} := \dfrac{U^{n+1} + U^n}{2}$, $t_{n+\frac{1}{2}} = \dfrac{t_{n+1} + t_n}{2}$

2. New relaxation-type numerical scheme: For $0 \le n \le N-1$,

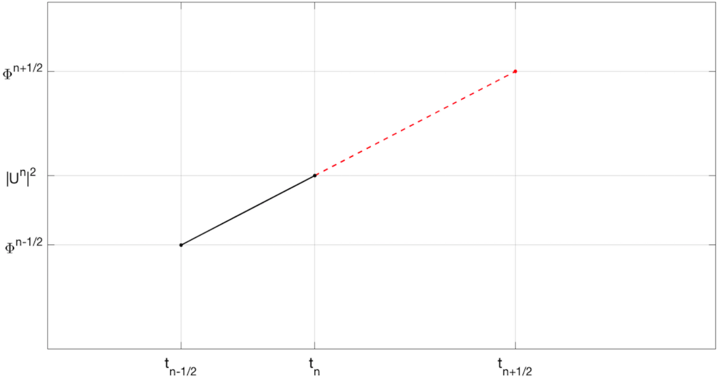
$$\begin{cases} \bar{\partial} U^n - \mathrm{i}\dfrac{\varepsilon}{2\alpha^2}\Delta U^{n+\frac{1}{2}} + \mathrm{i}\dfrac{\beta}{\varepsilon\alpha} V^{n+\frac{1}{2}} U^{n+\frac{1}{2}} = 0, \\ \Delta V^{n+\frac{1}{2}} = \Phi^{n+\frac{1}{2}}, \quad \Phi^{n+\frac{1}{2}} = \dfrac{k_n + k_{n-1}}{k_{n-1}} |U^n|^2 - \dfrac{k_n}{k_{n-1}} \Phi^{n-\frac{1}{2}}, \end{cases}$$

with $k_{-1} := k_0$, $U^0 = u_0$ and $\Phi^{-\frac{1}{2}} = |u_0|^2$

Motivation behind the relaxation scheme

- How do we approximate $\phi(t_{n+\frac{1}{2}})$?

  At step n, $\Phi^{n-\frac{1}{2}}$, U^n are known $\Rightarrow$ Compute $\Phi^{n+\frac{1}{2}}$ by *linear extrapolation* between $\Phi^{n-\frac{1}{2}}$ and $|U^n|^2$: $\Phi^{n+\frac{1}{2}} := \dfrac{k_n + k_{n-1}}{k_{n-1}}|U^n|^2 - \dfrac{k_n}{k_{n-1}}\Phi^{n-\frac{1}{2}}$



- Use $\Phi^{n+\frac{1}{2}}$ to obtain an approximation for v: $\Delta v = \phi \rightsquigarrow \Delta V^{n+\frac{1}{2}} = \Phi^{n+\frac{1}{2}}$

New relaxation-type scheme

❍ For $0 \le n \le N-1$,

$$\begin{cases} \Phi^{n+\frac{1}{2}} = \dfrac{k_n + k_{n-1}}{k_{n-1}} |U^n|^2 - \dfrac{k_n}{k_{n-1}} \Phi^{n-\frac{1}{2}}, \quad \Delta V^{n+\frac{1}{2}} = \Phi^{n+\frac{1}{2}}, \\ \bar{\partial} U^n - \mathrm{i} \dfrac{\varepsilon}{2\alpha^2} \Delta U^{n+\frac{1}{2}} + \mathrm{i} \dfrac{\beta}{\varepsilon\alpha} V^{n+\frac{1}{2}} U^{n+\frac{1}{2}} = 0, \end{cases}$$

with $k_{-1} := k_0$, $U^0 = u_0$ and $\Phi^{-\frac{1}{2}} = |u_0|^2$ (for now)

❍ INSPIRED BY:

- Besse (2004); Katsaounis & K. (2018); Besse, Descombes, Dujardin, Lacroix-Violet (2021)
- In Katsaounis & K. (2018) the *first* a posteriori error estimator was constructed for the NLS equation with power nonlinearity

❍ ADVANTAGES:

- Expected to be second order accurate
- *Explicit* with respect to the *nonlinearity* $\Rightarrow$ No need to solve a nonlinear equation to obtain the next approximation
- Satisfies a *discrete version* of mass & energy conservation

Conservation Laws

❍ Continuous conservation laws

- Mass conservation: $\mathcal{M}(t) = \mathcal{M}(0)$ with $\mathcal{M}(t) := \|u(t)\|^2$
- Energy conservation: $\|\mathcal{E}(t)\| = \|\mathcal{E}(0)\|$ with

$$\mathcal{E}(t) := \frac{\varepsilon^2}{\alpha}\|\nabla u(t)\|^2 - \beta\|\nabla v(t)\|^2 = \frac{\varepsilon^2}{\alpha}\|\nabla u(t)\|^2 + \beta \int_\Omega v(x,t)|u(x,t)|^2\,dx$$

❍ Discrete conservation laws

- Discrete mass conservation: $\mathcal{M}^n = \mathcal{M}^0$ with $\mathcal{M}^n := \|U^n\|^2$
- Non-standard discrete energy conservation: $\|\mathcal{E}^n\| = \|\mathcal{E}^0\|$ with

$$\mathcal{E}^n := \frac{\varepsilon^2}{\alpha}\|\nabla U^n\|^2 + \beta\left(2\int_\Omega V^{n-\frac{1}{2}}(x)|U^n(x)|^2\,dx + \|\nabla V^{n-\frac{1}{2}}\|^2\right)$$

  and constant time-steps

  - What happens for *variable* time-steps? It holds

$$\mathcal{E}^{n+1} = \mathcal{E}^n + \mathcal{R}^n \quad \text{with} \quad \mathcal{R}^n := \frac{\beta(k_n - k_{n-1})}{2(k_n + k_{n-1})} k_n \|\frac{\nabla V^{n+\frac{1}{2}} - \nabla V^{n-\frac{1}{2}}}{k_n}\|^2$$

Numerical verification of the discrete conservation laws

❍ TOY MODEL 1: Constant time-steps

- $d = 2,\ \Omega = (-1,1)^2,\ T = 3,\ \alpha = \beta = 5$
- $u_0(x,y) = \left(\sin\left(\frac{x}{\pi}\right) + \mathrm{i}\cos\left(\frac{y}{\pi}\right)\right)(1-x^2)(1-y^2)$
- spatial discretisation: linear FE, $h = 0.015625$, $k = 10^{-3}$
- $\mathcal{M}_e^n := |\mathcal{M}^n - \mathcal{M}(0)|, \quad \mathcal{E}_{e,gl}^n := |\mathcal{E}^n - \mathcal{E}(0)|$

	$\varepsilon = 1$		$\varepsilon = 0.1$		$\varepsilon = 0.01$	
t_n	$\mathcal{M}_e^n$	$\mathcal{E}_{e,gl}^n$	$\mathcal{M}_e^n$	$\mathcal{E}_{e,gl}^n$	$\mathcal{M}_e^n$	$\mathcal{E}_{e,gl}^n$
0	4.55e-15	2.39e-16	7.22e-16	2.58e-15	3.94e-15	9.57e-15
1	2.06e-14	3.29e-16	4.11e-15	1.39e-15	3.55e-15	1.60e-14
2	4.33e-14	1.75e-16	1.66e-15	2.36e-15	8.55e-15	1.54e-14
3	5.97e-14	3.03e-16	7.32e-15	2.01e-15	1.44e-14	2.56e-14

Table: Errors in the conservation laws.

❇ Conservation of discrete mass & energy up to double precision accuracy

Numerical verification of the discrete conservation laws

❍ Toy model 2: Variable time-step

- $d = 2,\ \Omega = (-1,1)^2,\ T = 2,\ \alpha = \beta = 5,\ \varepsilon = 0.01$
- $u_0(x,y) = \left(\sin\left(\frac{x}{\pi}\right) + \mathrm{i}\cos\left(\frac{y}{\pi}\right)\right)(1-x^2)(1-y^2)$
- spatial discretisation: cubic FE, $h = 0.015625$
- $[0,T] = \cup_{j=0}^{7}[T_j, T_{j+1}];\ T_j = j/4,\ 0 \le j \le 8$

  In each $[T_j, T_{j+1})$, $k_n = 1.25(j+1)\times 10^{-3}, 0 \le j \le 7$
- $\mathcal{M}_e^j := |\mathcal{M}^j - \mathcal{M}(0)|,\quad \mathcal{E}_{e,gl}^j := |\mathcal{E}^j - \mathcal{E}(0)|,\quad \mathcal{E}_{e,loc}^j := |\mathcal{E}^j - \mathcal{E}^{j-1}|$

T_j	k_{j-1}	k_j	$\mathcal{M}_e^j$	$\mathcal{E}_{e,gl}^j$	$\mathcal{E}_{e,loc}^j$	$\mathcal{R}^j$
0.25	1.250e-03	2.500e-03	2.99e-15	3.11e-15	2.88e-11	1.28e-11
0.50	2.500e-03	3.750e-03	7.54e-14	2.93e-11	1.92e-10	1.22e-10
0.75	3.750e-03	5.000e-03	9.30e-14	2.21e-10	6.09e-10	4.42e-10
1.00	5.000e-03	6.250e-03	1.07e-13	8.31e-10	1.40e-09	1.09e-09
1.25	6.250e-03	7.500e-03	1.23e-13	2.23e-09	2.69e-09	2.20e-09
1.50	7.500e-03	8.750e-03	1.28e-13	4.92e-09	4.66e-09	3.92e-09
1.75	8.750e-03	1.000e-02	1.39e-13	9.59e-09	7.37e-09	6.32e-09
2.00	1.000e-02	–	1.41e-13	1.70e-08	–	–

Table: Errors in the conservation laws: variable time-step

New relaxation-type scheme: EOC

❍ TOY MODEL 3:

- $d = 2,\ \Omega = (-1,1)^2,\ T = 1,\ \alpha = \beta = \varepsilon = 1$
- $v(x,y,t) = \mathrm{e}^{-t} \sin\left(\pi(x^2-1)(y^2-1)\right),\ u(x,y,t) = (1+\mathrm{i})v(x,y,t)$ and appropriate right-hand side in the SPS
- spatial discretisation: FE with polynomial degree $r = 9,\ h = 0.0625$
- $e(u;k) := \max\limits_{0\le n\le N} \|u(\cdot,t_n) - U^n\|, \quad e(v;k) := \max\limits_{0\le n\le N} \|v(\cdot,t_n) - V^n\|$

k	$e(u;k)$	Rate	$e(v;k)$	Rate
0.04	3.72233e-4	-	9.60801e-4	-
0.02	9.49430e-5	1.971	2.51017e-4	1.936
0.01	2.39046e-5	1.990	6.41950e-5	1.967

Table: Temporal experimental orders of convergence.

Generalisation: SPS with time-dependent coefficients

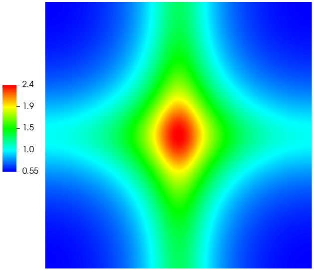
$$\begin{cases} \partial_t u - \mathrm{i}p(t)\Delta u + \mathrm{i}q(t)vu = 0 & \text{in } \Omega\times(\tau, T), \\ \Delta v = |u|^2 - \mu & \text{in } \Omega\times(\tau, T), \\ u(x,\tau) = u_0(x) & \text{in } \Omega, \\ \{\mu = 0 \text{ and } u = v = 0\}, \quad \text{OR} \quad \{\mu = \|u_0\|_{L^2}^2 \text{ and } u, v \text{ periodic}\} & \text{on } \partial\Omega\times(\tau, T], \end{cases}$$

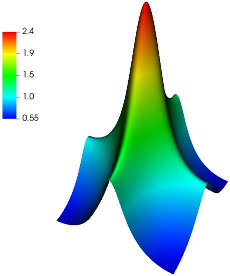
- The above SPS satisfies the following energy balance law
  $p(t)\dfrac{d}{dt}\mathcal{E}_k(t) - \dfrac{q(t)}{2}\dfrac{d}{dt}\mathcal{E}_v(t) = 0$ (instead of the energy conservation)
- Our new relaxation-type scheme satisfies a discrete version:
  $p(t_{n-\frac{1}{2}})\bar{\partial}\mathcal{E}_k^n - \dfrac{q(t_{n-\frac{1}{2}})}{2}\bar{\partial}\mathcal{E}_v^n = 0$

❍ More details can be found in A. Athanasoulis, Th. Katsaounis, I.K., S. Metcalfe, *"A novel, structure-preserving, second-order-in-time relaxation scheme for Schrödinger-Poisson systems"*, J. Comput. Phys. 490 (2023)

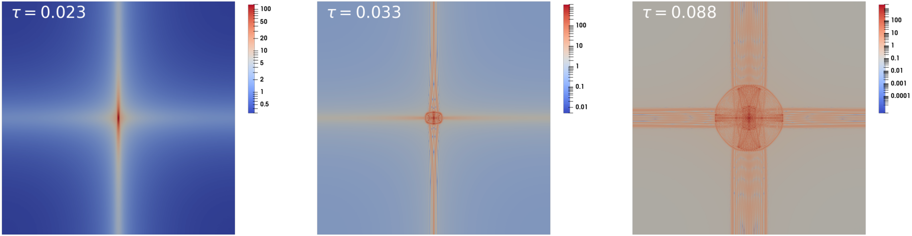
A Cosmological Example: "Sine Wave Collapse"

- $d = 2$, $\Omega = (-0.5, 0.5)^2$, $\tau = 0.01$, $T = 0.088$, $\mu = \|u_0\|^2 = 1$
- $p(t) = \dfrac{\varepsilon}{2t^{3/2}}$, $q(t) = \dfrac{\beta}{\varepsilon t^{1/2}}$, $\beta = 1.5$, $\varepsilon = 6 \times 10^{-5}$
- Spatial discretisation via linear FE, $k = 5 \times 10^{-5}$
- Initial density $|u_0|^2$:

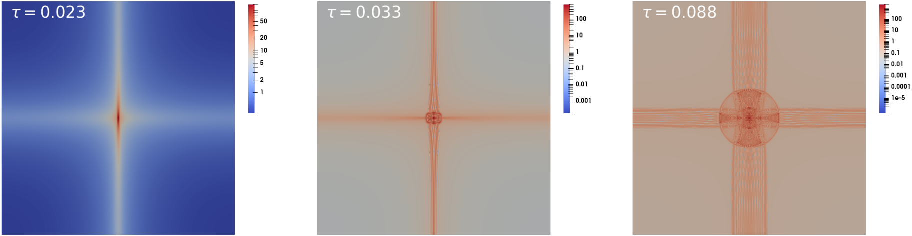




“Sine Wave Collapse”: Simulations



Numerical density $|U^N|^2$ (logarithmic scale) at $t_n = 0.0023, 0.033, 0.088$: 1024×1024 grid



Numerical density $|U^N|^2$ (logarithmic scale) at $t_n = 0.0023, 0.033, 0.088$: 2048×2048 grid

A posteriori estimates

❍ *What is an a posteriori estimate?* If U is a numerical approximation to u, then for some norm $\|\cdot\|_A$,

$$\|u - U\|_A \leq \eta(U) \tag{1}$$

- $\eta(U)$: *computable quantity* depending *only* on U and the data of the problem
- $\eta(U)$: decreases with *optimal order* (i.e., converges with the same order as the numerical method)

❍ ADVANTAGES

1. Error control through a posteriori estimates provide mathematical guarantees on how accurate the approximate solution is

$$\Downarrow$$

Provide *reliable* numerical computations

2. $\eta(U) = \sum_i \eta_i(U)\Delta x_i + \sum_j \eta_j(U)\Delta t_j$ gives an understanding *where the error is coming from* $\rightsquigarrow$ Construction of adaptive algorithms

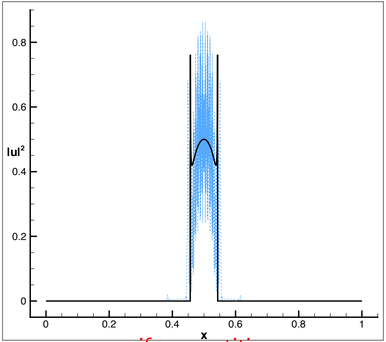
3. A posteriori error control is a way to overcome the limitations of ad hoc adaptivity

Adaptivity

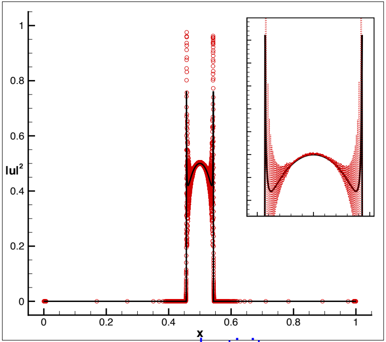
❍ What is an *adaptive algorithm?* Construction of *non-uniform grids* in a *systematic way*

❍ Essential tool for:

1. Detecting regions where the solution exhibits *singular behaviour* (e.g., blowup, caustics, boundary layers)
2. Capturing disparate space-time scales *efficiently* (e.g., fluid structure interaction)
3. Adaptive algorithms typically lead to *reduced* computational cost



...uniform partition



...adaptivity

A posteriori error control: Reconstruction Technique

(Akrivis, Makridakis & Nochetto, 2005)

- Aim: Derivation of optimal order a posteriori error estimates for the new relaxation-type scheme for both u (in the $L^\infty(L^2)-$norm) and v ($L^\infty(H^1)-$norm)

- New relaxation-type scheme is *second order accurate*

- The equation for the potential *does not include* any time-derivative ✓

- $U(t) := \ell_0^n(t)U^n + \ell_1^n(t)U^{n+1},\ t \in I_n,\ \ell_0^n(t) := \dfrac{t_{n+1} - t}{k_n},\ \ell_1^n(t) := \dfrac{t - t_n}{k_n}$
  - Using U in the a posteriori error analysis leads to suboptimal bounds (Dörfler, 1996)
  - Introduce a *reconstruction* $\hat{U}$ of U, work with $u - U = (u - \hat{U}) + (\hat{U} - U)$

Reconstruction Technique: Main idea

1. Find a *continuous* projection or interpolant $\hat{U}$ of U
2. $\hat{U} - U$ is of optimal order
3. $\hat{U}$ satisfies a perturbation of the original PDE
4. The perturbation term (residual) is a computable quantity or can be estimated by computable quantities of optimal order of accuracy
5. Use PDE stability arguments to obtain the final a posteriori estimates

A posteriori error control: Reconstruction Technique

- $U(t)$ & $V(t)$, $t \in I_n$: linear interpolants between U^n, U^{n+1} & V^n, V^{n+1}
  - Using U in the a posteriori error analysis $\Rightarrow$ first order bounds (Döfler, 1996)
  - Introduce a *reconstruction* $\hat{U}$ of U; work with $(u - \hat{U}) + (\hat{U} - U)$ (Akrivis, Makridakis & Nochetto, 2005)

New relaxation-type scheme reconstruction & its properties

For $0 \le n \le N-1$ and $t \in I_n$,

$$\hat{U}(t) := U^n + \mathrm{i}\frac{\varepsilon}{2\alpha^2}\int_{t_n}^{t} \Delta U(s)\,ds - \mathrm{i}\frac{\beta}{\varepsilon\alpha}\int_{t_n}^{t} \mathcal{I}_{n+\frac{1}{2}}(VU)(s)\,ds,$$

with $\mathcal{I}_{n+\frac{1}{2}}$ the linear interpolant of VU at $t_n, t_{n+\frac{1}{2}}$

PROPERTIES:

1. $\hat{U}$ is a time-continuous function; $\hat{U}(t_n) = U(t_n) = U^n$
2. $\hat{U} - U$ is second order accurate
3. $\partial_t \hat{U} - \mathrm{i}\frac{\varepsilon}{2\alpha^2}\Delta\hat{U} + \mathrm{i}\frac{\beta}{\varepsilon\alpha}V\hat{U} = \hat{r}_1$ and $\Delta V - |\hat{U}|^2 = \hat{r}_2$ in I_n, with the residuals $\hat{r}_1$, $\hat{r}_2$ *computable* and of second order

An a posteriori error estimate

For $d = 1, 2$ and $0 \le n \le N - 1$ and $t \in I_n$, it holds

$$\|(u - \hat{U})(t)\| \le \eta(t) \qquad \text{and}$$
$$\|\nabla(v - V)(t)\| \le \mathcal{H}(\hat{U}, u_0; t)\eta(t) + \|\hat{r}_2(t)\|,$$

with

$$\eta(t) := \exp\left(\frac{|\beta|}{\varepsilon\alpha}\int_{t_n}^{t}\mathcal{H}(\hat{U}, u_0; \tau)\|\hat{U}(t)\|_{L^\infty}\,d\tau\right)$$
$$\times\left(\|(u - \hat{U})(t_n)\| + \int_{t_n}^{t}\left(\frac{|\beta|}{\varepsilon\alpha}\|\hat{U}(\tau)\|_{L^\infty}\|\hat{r}_1(\tau)\|_{H^{-1}} + \|\hat{r}_2(\tau)\|\right)d\tau\right)$$

and $(u - \hat{U})(0) = 0$

- PROOF: ...Very Technical!...
- MAIN INGREDIENTS:
  1. Energy techniques for the continuous problem
  2. Continuous mass & energy conservation
  3. Gagliardo-Nirenberg inequality
  4. Sobolev embeddings + H^2-regularity estimate for the Poisson equation

A numerical implementation: EOC of the residuals

- $d = 1,\ [a, b] = [-1, 1],\ T = 1, \alpha = \beta = 1\ \varepsilon = 0.1$
- B-splines of degree 3, 1000 grid points
- $v(x, t) = \mathrm{e}^t (1 - x^2)^3 \sin(\pi(1 - x^2)), \quad u(x, t) = (1 + \mathrm{i}) v(x, t)$
- For $\|\hat{r}_1(t)\|$:

k	$\int_{t_{N-1}}^{T} \|\hat{r}_1(\tau)\|\, d\tau$	Rate	$\int_0^T \|\hat{r}_1(\tau)\|\, d\tau$	Rate
1.00e-4	7.58e-6	–	2.67e-4	–
8.00e-3	4.62e-6	2.218	1.70e-4	2.017
4.00e-3	4.80e-7	3.267	4.20e-5	2.020
2.00e-3	5.98e-8	3.005	1.04e-5	2.009
1.00e-3	7.46e-9	3.002	2.60e-6	2.004
8.00e-4	3.82e-9	3.002	1.66e-6	2.003

- For $\|\hat{r}_2(t)\|$:

k	$\int_{t_{N-1}}^{T} \|\hat{r}_2(\tau)\|\, d\tau$	Rate	$\int_0^T \|\hat{r}_2(\tau)\|\, d\tau$	Rate
1.00e-4	9.60e-6	–	2.94e-4	–
8.00e-3	4.90e-6	3.009	1.87e-4	2.031
4.00e-3	6.08e-7	3.010	4.60e-5	2.020
2.00e-3	7.58e-8	3.004	1.14e-5	2.008
1.00e-3	9.47e-9	3.002	2.87e-6	1.995
8.00e-4	4.85e-9	3.000	2.85e-6	1.980

Ongoing & Future Work

1. A posteriori error analysis for *fully discrete schemes*

2. Further numerical implementations

3. A posteriori error estimates for $d = 3$ (other Sobolev embedding inequalities)

4. Design of adaptive algorithms, based on the a posteriori error estimators

5. Extension of the a posteriori error analysis and adaptivity to SPS with time-dependent coefficients

6. Higher order time-discretisations???

Thank you very much!