Finding Stationary Solutions with Constraints using Damped Dynamical Systems

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Motivation

It is generally challenging to find solutions to non-linear equations. Comsol built-in stationary solvers sometimes fails and also require good initial guesses. Yet, this situation occurs in multiple applications in science and technology. Adding constraints on the solution implies further difficulties for numerical methods.

The Dynamical Functional Particle Method (DFPM)

Consider the abstract equation for an unknown v, $\min_v E(v)$,

$$\mathcal{F}(v) = -\delta E(v)/\delta v = 0.$$

We introduce a parameter τ and define a new time dependent differential equation, such that $u \to v$ when $\tau \to \infty$,

$$u_{\tau\tau} + \eta u_\tau = \mathcal{F}(u).$$

We recognize a second-order damped system where η represents the damping. However, the method is suitable for problems far from this mechanical analogue [1].

Stationary Solutions to the Heat Equation

We consider heat transport, including non-linear source terms

$$\rho c_p u_t = \nabla \cdot (k \nabla u) + F(\boldsymbol{r}, t).$$

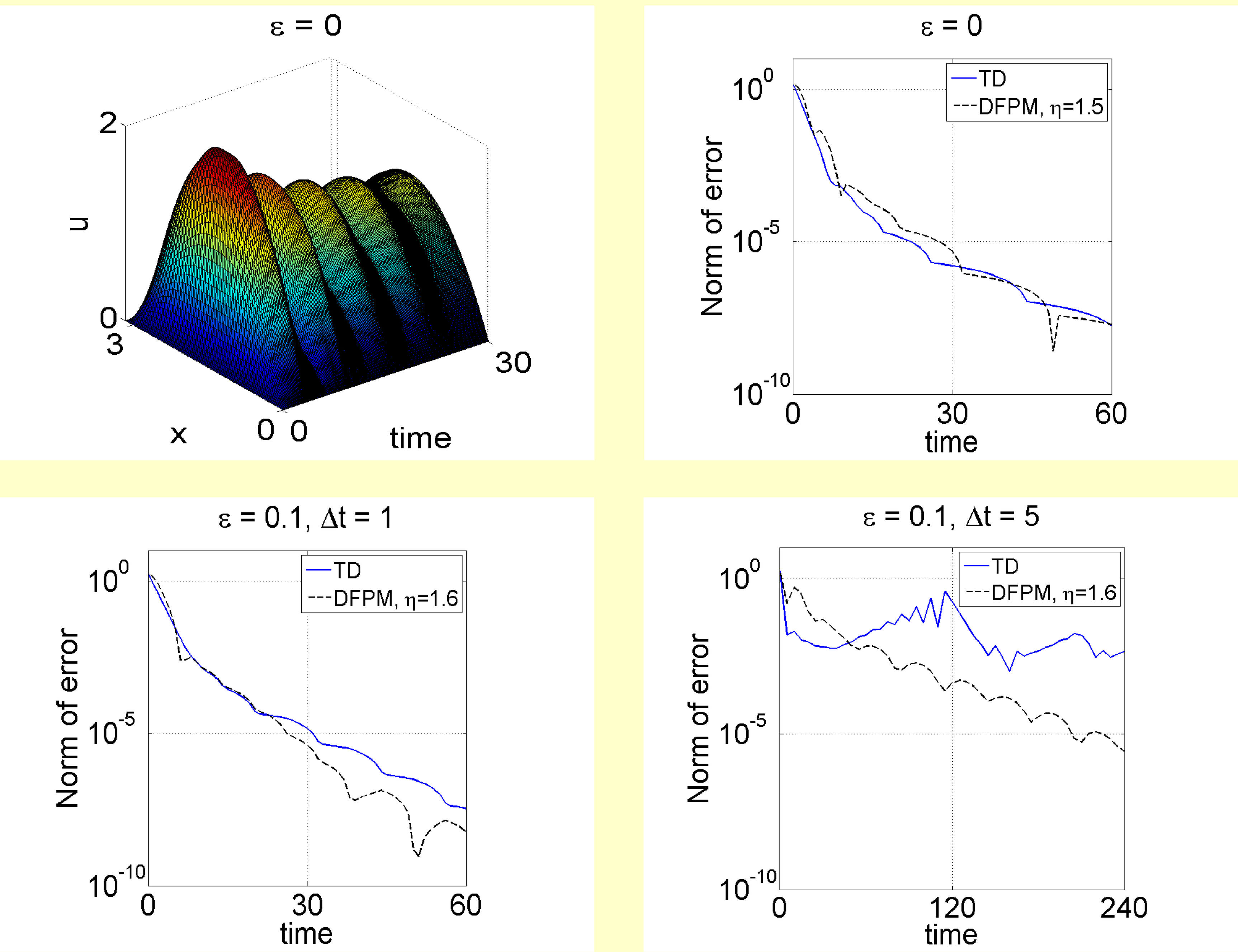
With Dirichlet boundary conditions and the physical parameters set to unity, we study the following Time Dependent (TD) dimensionless, non-linear equation in terms of stationary solutions,

$$u_t = u_{xx} + 1 + \varepsilon u^2.$$

The linear ($\varepsilon = 0$) problem have a simple analytic stationary solution. We then ($\varepsilon \neq 0$) compare with the built-in stationary solvers in Comsol [2]. Applying the DFPM we have

$$u_{\tau\tau} + \eta u_\tau = u_{xx} + 1 + \varepsilon u^2.$$

Convergence to the Stationary Solutions



Constraints

The DFPM can be used for additional constraints, $G_j(u) = 0$,

$$u_{\tau\tau} + \eta u_\tau = \mathcal{F}(u) + \sum_j \lambda_j \mathcal{G}_j(u),$$

where λ_j are Lagrange multiplicators and

$$\mathcal{G}_j(u) = \delta G_j(u)/\delta u,$$

are defined by the functional derivative of a constraint functional [3].

Non-linear Schrödinger Equation (NLSE)

In modern physics, the stationary NLSE may have the form

$$-\frac{\hbar^2}{2M}\nabla^2\varphi + U_0 |\varphi|^2 \varphi = \mu\varphi,$$

for the complex wavefunction φ. Which is constrained by the normalization condition

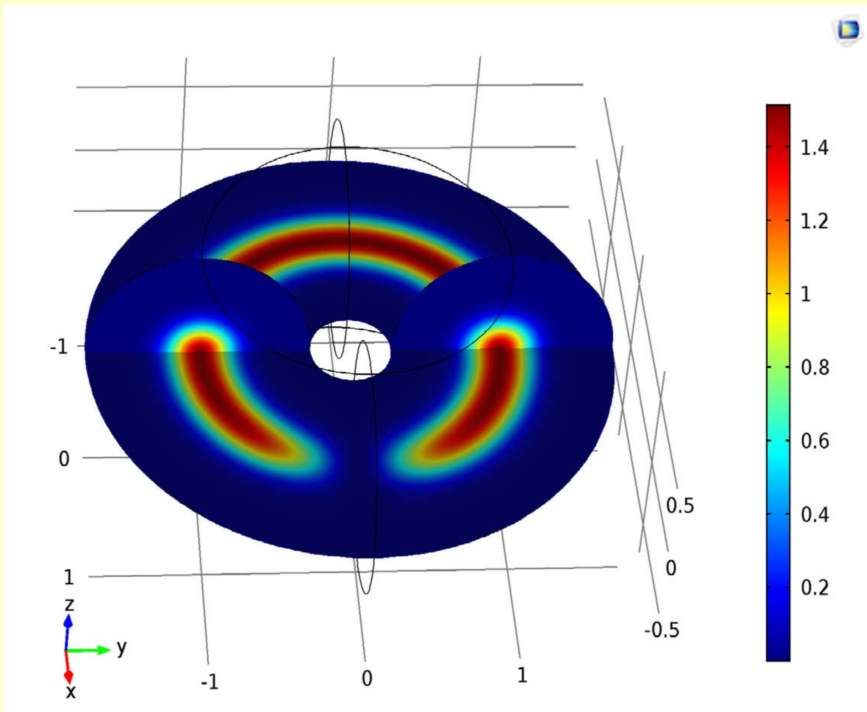
$$\int |\varphi|^2 \, dV = N_\varphi,$$

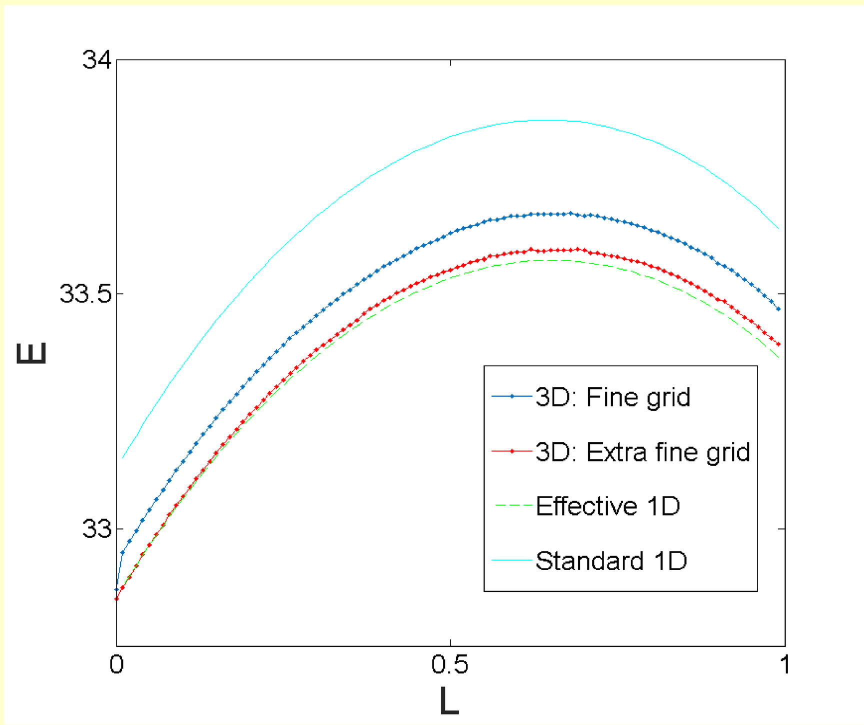
where N_φ is the number of atoms, M is the mass of an atom, and the atom-atom mean field interaction parameter U_0 can be varied in sign and amplitude. We recently solved this problem with DFPM for a ring geometry [3].

Future Work

In an ongoing project we use Comsol to investigate more realistic geometries [4].

Example of a dark soliton in a torus-shaped 3D Bose-Einstein condensate (BEC).





The energy, E, of the BEC, given a normalization constraint and an additional constraint on the angular momentum, L.

Can we implement DFPM efficiently in Comsol to find stationary solutions with constraints?

References

[1] S. Edvardsson, M. Gulliksson and J. Persson, J. Appl. Mech. **79**, 021012 (2012).
[2] www.comsol.com. We are using *Comsol 5.2.*
[3] P. Sandin, M. Ögren and M. Gulliksson, Phys. Rev. E **93**, 033301 (2016).
[4] P. Sandin, *Dimensional reduction in Bose-Einstein condensed clouds of atoms in tight potentials of any geometry and any interaction strength,* to be submitted.

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