Finding Stationary Solutions of PDEs with Constraints using Damped Dynamical Systems

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Abstract

The dynamical functional particle method (DFPM) is a method for solving equations, e.g. PDEs, using a second order damped dynamical system. We show how the method can be extended to include constraints both explicitly as global constraints and adding the constraints as additional damped dynamical equations. These methods are implemented in Comsol and we show numerical tests for finding the stationary solution of a nonlinear heat equation with and without constraints (global and dynamical). The results show that DFPM is a very general and robust way of solving PDEs and it should be of interest to implement the approach more generally in Comsol.

Keywords: PDE, constraints, dynamical system

Introduction

Consider a general time independent PDE as the abstract equation

$$F(u) = 0. \qquad (1)$$

A well-known strategy to solve (1) is to introduce a (artificial) time-variable τ and reformulate the problem as $u_\tau = F(u)$ giving the required stationary solution $F(u) = 0$ when $\tau \to T, T \leq \infty$. The dynamical functional particle method (DFPM) uses instead a damped second order dynamical system

$$mu_{\tau\tau} + \eta u_\tau = F(u), \qquad (2)$$

to solve (1). The mass, $m > 0$, and damping parameter, $\eta > 0$, is optimized for fast convergence [1]. For a conservative system where $F(u)$ has a convex potential $V(u)$, global convergence can be guaranteed. By using a symplectic solver, see [5], it has been shown that DFPM has extraordinary convergence and accuracy properties, see [1, 2].

In this paper we extend DFPM to include constraints

$$G_j(u) = 0, j = 1, \ldots, k.$$

When adding constraints we reformulate the setting and assume that there exist a minimization formulation $\min_u V(u)$ with $G_j(u) = 0$ and $F(u) = -\delta V/\delta u$, where δ denotes functional derivatives. Define the functional $L(u) = V(u) + \sum_j \lambda_j G_j$ where λ_j are the Lagrange multipliers then the dynamical functional particle method with constraints is

$$mu_{\tau\tau} + \eta u_\tau = F(u) + \sum_j \lambda_j \delta G_j/\delta u. \qquad (3)$$

However, from experience the value of the damping η is not of crucial importance.

We consider the problem of solving for the stationary solution of a nonlinear PDE with additional constraints either given by a time dependent problem or by extending to a(n) (artificial) time dependent problem. We also tested Comsol's built-in stationary solvers, however, they may fail to find a solution if the initial guess is inadequate and this motivates our study.

Use of COMSOL Multiphysics® Software

We have used the General Form PDE Physics Interface [3]. For the heat equation we first used a time-dependent solver with Dirichlet boundary conditions on a finite line with the initial conditions being zero. Then we changed to periodic boundary conditions and added, in different ways, a constraint on the solution.

In the absence of a symplectic solver in Comsol, we have used the generalized α-solver.

Results

In the following we report on numerical experiments. In Figure 1 we illustrate the exponentially oscillatory convergence behavior of

DFPM for the inhomogeneous stationary heat equation where $F(u) = u_{xx} + 1, u(0,t) = u(\pi,t) = 0, u(x,0) = 0$.

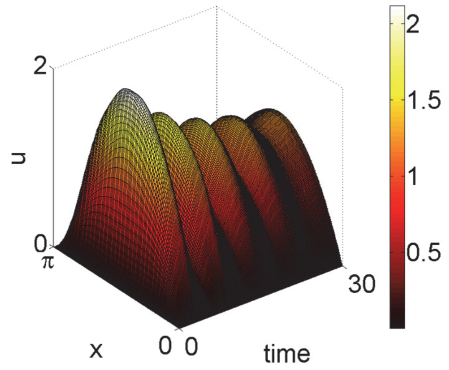

Figure 1. Oscillatory convergence of DFPM, $\boldsymbol{\epsilon = 0}$.

We then compare the convergence of the time dependent (TD) heat equation with DFPM, as well as the Comsol built-in stationary solvers (SS) applied to the time-dependent nonlinear heat equation

$$u_t = u_{xx} + 1 + \epsilon u^2, \qquad (4)$$

with initial and boundary conditions as before. We use the discrete L_2-norm to calculate the norm of the error. Define $e_j(x_i) = u(x_i, t_j) - u_{SS}(x_i)$ as the error between the numerical solution and the stationary solution for some fixed large time t_j, where u_{SS} is the stationary solution. Then we define the error at time t_j as

$$error_j = \sqrt{\sum_i |e_j(x_i)|^2 \Delta x},$$

where Δx is the size of the discretization in space. From Figure 2, where $\epsilon = 0.1$, we can see that DFPM is roughly converging as fast as the TD.

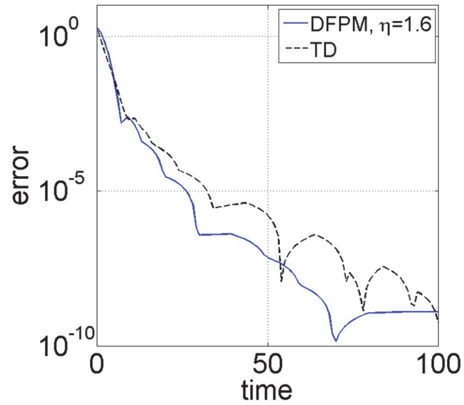

Figure 2. Comparison with the TD heat equation (4) (no constraint), $\epsilon = 0.1, \Delta t = \Delta\tau = 1$.

However, in Figure 3, for a larger time step and $\epsilon = -1$, TD diverges but DFPM is still stable. Hence, this is an example that further shows the versatility of DFPM.

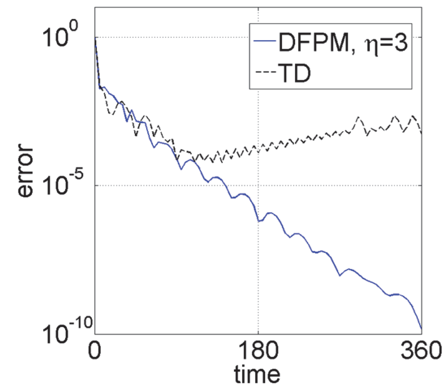

Figure 3. Comparison with the TD heat equation (4) (no constraint), $\epsilon = -1, \Delta t = \Delta\tau = 5$.

Let us now consider (4) with periodic boundary condition $u(0,t) = u(\pi,t)$ and the constraint

$$G(u) = \int_0^\pi u \, dx - 1 = 0. \qquad (5)$$

Using (3) we get DFPM in the form

$$mu_{\tau\tau} + \eta u_\tau = u_{xx} + 1 + \epsilon u^2 + \lambda\pi. \qquad (6)$$

In order to obtain an expression for the Lagrange multiplier λ, we make the following ansatz for the constraint (3)

$$mG_{\tau\tau} + \eta G_\tau = -kG, \; k > 0 \qquad (7)$$

Note that the damping, η, in (7) is the same as in DFPM but the dynamical behavior of (7) may be different through the parameter k. After some algebra we obtain from (5)-(7) that

$$\lambda = \frac{1}{\pi^2}\left[k - \int_0^\pi (u_{xx} + ku + \epsilon u^2)dx - \pi\right]. \quad (8)$$

We solve the two coupled damped systems (6), (7) in Comsol for different values of η and k in order to study the convergence properties. We denote this approach by DFPML, where L refers to the Largrange formulation. This gives the same solution for $\tau \to \infty$ as the built in stationary solver with the constraint implemented as a standard Global Constraint. The numerical result for three different values of k is shown in Figure 4.

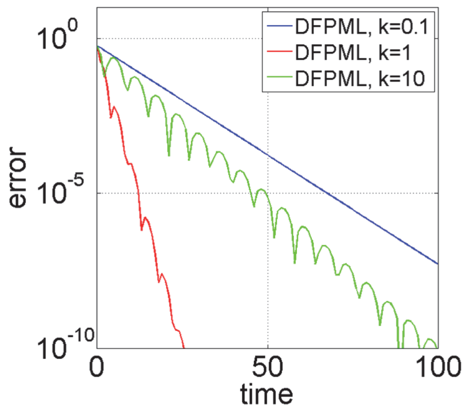

Figure 4. Convergence in DFPML with the constraint implemented with different k. Parameters: $\boldsymbol{\epsilon} = \mathbf{0.1}, \boldsymbol{\Delta\tau} = \mathbf{1}, \boldsymbol{m} = \mathbf{0.1}, \boldsymbol{\eta} = \mathbf{2}\sqrt{\boldsymbol{m}}$.

The choice of the damping $\eta = 2\sqrt{m}$ is according to the linear analysis presented in [1]. In Figure 5 it is shown that the convergence is fairly robust with respect to the choice of k.

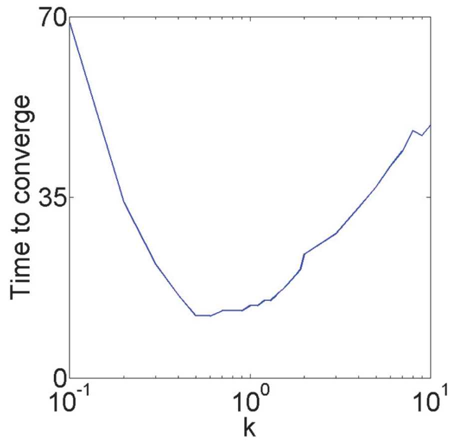

Figure 5. Time in $\boldsymbol{\tau}$ for DFPML to converge within 5 decimals to the stationary solution for different values of k. Parameters: $\boldsymbol{\epsilon} = \mathbf{0.1}, \boldsymbol{\Delta\tau} = \mathbf{1}, \boldsymbol{m} = \mathbf{0.1}, \boldsymbol{\eta} = \mathbf{2}\sqrt{\boldsymbol{m}}$.

For an additional comparison, we solve the TD heat equation

$$u_t = u_{xx} + 1 + \epsilon u^2 + \lambda\pi, \quad (9)$$

with the corresponding ansatz, $G_t = -kG,\ k > 0$, for the constraint (5). We denote this method as TDL. In this case, the expression for the Lagrange multiplier λ can be shown to be given again by (8) and the stationary solution to (6) and (9) is just a constant which we use to calculate the error of the different methods. In addition to the two methods TDL and DFPML, we denote the TD and DFPM with the constraint instead beeing implemented as a Global Constraint in Comsol as TDGC and DFPMGC. As can be seen in Figure 6, the implementation with a Lagrange multiplier λ (DFPML and TDL) has far better convergence properties.

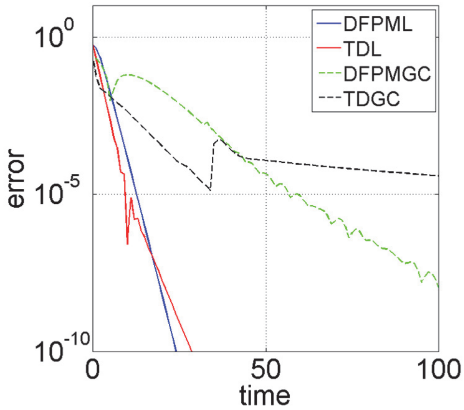

Figure 6. For time-dependent problems with a constraint, the exponential constraint formalism, $\boldsymbol{\lambda(u)}$, outperform the Comsol built in integral (Global Constraint). Parameters: $\boldsymbol{\epsilon = 0.1, \Delta t = \Delta\tau = 1,}$ $\boldsymbol{k = 1, m = 1, \eta = 2}$.

Also, the choice of η and m can be further tuned such that DFPM performs even better, see Figures 7 and 8.

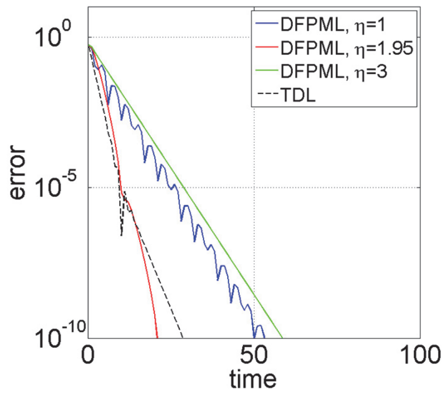

Figure 7. By using an optimal $\boldsymbol{\eta}$, DFPML can outperform TDL. Parameters: $\boldsymbol{\epsilon = 0.1,}$ $\boldsymbol{\Delta t = \Delta\tau = 1, k = 1, m = 1}$.

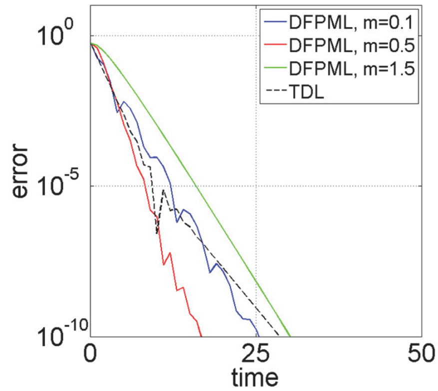

Figure 8. By optimize also the mass, $\boldsymbol{m}$, DFPML perform even better. Parameters: $\boldsymbol{\epsilon = 0.1, \Delta t = \Delta\tau =}$ $\boldsymbol{1, k = 1, \eta = 2\sqrt{m}}$.

Conclusions

We have shown that Comsol implementations of DFPM successfully finds the stationary solutions to non-linear problems with constraints [4]. In our future work we want to use symplectic methods in Comsol which may improve the results of DFPM such that it can be the first choice in Comsol simulations of this kind.

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