The Dynamical Functional Particle Method
A method for solving constrained optimization problems using damped dynamical systems

Mårten Gulliksson, Magnus Ögren, and Patrik Sandin
University of Örebro, Unit of Mathematics, Sweden
marten.gulliksson@oru.se

Abstract
The Dynamical Particle Functional Method (DPFM) is a method for solving equations by using a damped second-order dynamical system. The dynamical system is solved by a symplectic method that is especially tailored for conservative systems. In this work we have extended DPFM to include constraints either as additional damped dynamical systems or using projections.

Introduction
The idea behind DPFM is to solve \( F(u) = 0 \) by solving a damped second order dynamical system
\[
\ddot{u} + \rho \dot{u} = F(u)
\]
such that \( \lim_{\text{iter} \to \infty} F(u) = 0 \). The damping parameter \( \rho > 0 \). It can be proven that if there is a convex potential \( V(u), F = -\nabla V \) then DPFM will converge to
\[ \min_{u \in \mathbb{R}^n} V(u) \]
i.e. \( \nabla V = -F = 0 \). Here, we generalize DPFM to include constraints, i.e.,
\[ \min_{u \in \mathbb{R}^n} V(u) \text{ s.t. } g(u) = 0 \]
(1)
where \( g : \mathbb{R}^n \to \mathbb{R}^m \). We will assume that (1) is convex.

What makes DPFM attractive is the use of simple symplectic methods. The damping parameter can be chosen, analytically or numerically, to get an optimal local convergence rate.

Projection
Necessary condition for (1) having a local minimum is
\[ \nabla^2 V(u) = \left( I - \nabla g(u)^T \nabla g(u)^T \right) \nabla V(u) = 0 \]
where \( P \) is the projection on the tangent space of \( \{ v : g(v) = 0 \} \). DPFM is then
\[ \ddot{u} + \rho \dot{u} = -\left( I - \nabla g(u)^T \nabla g(u)^T \right) \nabla V(u). \]
(2)

Theorem 1. For a convex minimization problem DPFM for (2) is asymptotically convergent.

Lagrange formulation
Define the Lagrange function of (1) as
\[ L(u, \mu) = V(u) + g(u)^T \mu, \]
where \( \mu \) is a vector with the Lagrange parameters. The first order condition for a minimum is
\[ \nabla L(u, \mu) = \nabla V(u) + \nabla g(u)^T \mu = 0, \quad g(u) = 0 \]
where \( \nabla g(u) = (\nabla g_1(u), \ldots, \nabla g_m(u)) \). We formulate DPFM based on the dynamical system
\[ \ddot{u} + \rho \dot{u} = -\nabla V(u) - \nabla g(u)^T \mu. \]
(3)
Additionally, we need to fulfill the constraints \( g(u) = 0 \) and this can be done either by projection or solving second order damped constraint equations.

Projection - Shake and Rattle
This approach has been developed for non-damped systems, see [2, 3]. For the use in DPFM we refer to [1] for the solution of the nonlinear Schrödinger equation. For this approach we have the

Theorem 2. For a convex minimization problem (1) DPFM is asymptotically convergent.

Damped constraints
Damping equations for the constraints
\[ \dot{\dot{u}} + \dot{\mu} = -\dot{\mu}, \quad \dot{\mu} = 0, \]
give the Lagrange parameters as
\[ \nabla g_j(u)^T \nabla g_j(u) \mu_j = K \mu_j - \nabla g_j(u)^T \nabla V(u) - h_j(u), \quad \mu_j = 0, \]
where \( K = \text{diag}(K_1, \ldots, K_m) \) the efficiency parameter for constraints.

Theorem 3. For a convex minimization problem (1) DPFM is locally asymptotically convergent.

Symplectic Euler
From (3) we have
\[ u = v, \quad \dot{v} = -\nabla V - \nabla g(u)^T \mu, \]
Symplectic Euler with constant time step \( \Delta t \) and damping parameter \( \eta \) is
\[ u_{k+1} = u_k + \Delta t v_k, \quad v_{k+1} = v_k + \Delta t (-\nabla V(u_{k+1}) - \nabla g(u_{k+1}) \mu_k + \Delta t \eta \mu_k). \]

Results for the linear eigenvalue Problems
Consider the eigenvalue problem \( Au = \lambda u, u^T u = 1 \) where \( A \in \mathbb{R}^{n \times n} \) is positive definite. Assume \( 0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n \).
\[ \min_{\|u\| = 1} \langle \lambda u, u \rangle = \lambda_1 \]
is the eigenvalue \( \lambda_1 \) corresponding to the smallest eigenvalue \( \lambda_1 \). The rest of the spectrum can be attained by adding constraints \( u^T u = \eta \), where \( \eta > 0 \), to get
\[ \min_{\|u\| = 1} \langle \lambda u, u \rangle + \rho \|u\|^2 \]
with convergence as below.

Rest of the spectrum - additional orthogonality constraints
Solving for the second eigenvalue and eigenvector
\[ u_1 = \frac{1}{\sqrt{\lambda_1}} \left( 1, 0, \ldots, 0 \right), \]
where the convergence results are shown below.

Conclusions
- DPFM is a very general approach for solving nonlinear convex problems with nonlinear constraints
- Convergence is exponential when using symplectic solvers
- Can compete with state-of-the-art solvers for linear eigenvalue problems

Forthcoming research
We believe that the true advantage of DPFM is for highly nonlinear problems where standard methods fail. This will require a systematic way of choosing damping parameters and time step in the symplectic solver at each iteration step.

References