Solving Constrained Optimization Problems Using Damped Dynamical Systems

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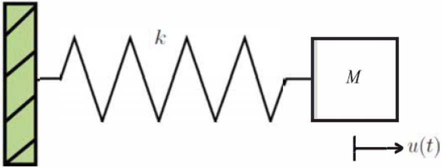
Brief outline of the talk

- Intro to the method using second-order damped dynamical system in fictitious time for constrained minimization
- A simple example of explicit solution of a (fictitious time dependent) Lagrange multiplier
- Intro to some of the applications we have used the method for

Intro

The dynamical functional particle method (DFPM) with dynamical constraints:

- Main principal of the DFPM, second-order in fictitious time, mechanical analog: a damped spring system 

- Main principal of the dynamical constraints, also second-order in fictitious time!
- Explicit solution of the (fictitious time dependent) Lagrange multipliers

We have demonstrated the efficiency and practical implementation of the method for several different (non-linear) problems.

DFPM is readily extended to more general constrained problems. Here we consider a convex minimization problem for $E(u)$ with smooth constraint functionals $G_j(u) = 0$, i.e.

$$\min_u E(u), \quad \text{s.t.} \;\; G_j(u) = 0. \quad (11)$$

Define the constrained energy functional (Lagrange functional) as

$$I(u, \mu_1, \mu_2 \ldots) = E(u) + \sum_j \mu_j G_j(u)$$

Then the problem has a unique solution u^* if

$$\frac{\delta E}{\delta \bar{u}} + \sum_j \mu_j \frac{\delta G_j}{\delta \bar{u}} = 0$$

and $\delta G_j / \delta \bar{u}$ are linearly independent at u^*

Dynamical System Formulation

The following damped dynamical system has u^* as a stationary solution

$$\ddot{u} + \eta \dot{u} + \frac{\delta E}{\delta \bar{u}} + \sum_j \mu_j \frac{\delta G_j}{\delta \bar{u}} = 0 \quad (12)$$

The Lagrange parameters can be found by defining additional damped systems for the constraints.

Damped Approach

Additional dynamical system for the constraints G_j are defined as

$$\ddot{G}_j + \eta \dot{G}_j + k_j G_j = 0, \quad \eta > 0,\ k_j > 0$$

- $G_j(u(\tau))$ tends to zero exponentially fast as τ tends to ∞
- Can be used to derive expressions for the Lagrange multipliers $\mu_j(\tau)$

Let's give a very simple example...

Normalization Constraint

Normalization constraint

$$G_1 = 1 - \int |u|^2 \mathrm{d}\mathbf{r} = 0$$

with first- and second-order derivatives

$$\dot{G}_1 = -\int \left(\dot{\bar{u}} u + \bar{u}\dot{u}\right) \mathrm{d}\mathbf{r}, \qquad \ddot{G}_1 = -\int \left(\ddot{\bar{u}} u + 2\dot{\bar{u}}\dot{u} + \bar{u}\ddot{u}\right) \mathrm{d}\mathbf{r}$$

After simplification

$$\ddot{G}_1 + \eta \dot{G}_1 = -\int \left(\left\{\ddot{\bar{u}} + \eta\dot{\bar{u}}\right\} u + \bar{u}\left\{\ddot{u} + \eta\dot{u}\right\} + 2|\dot{u}|^2\right) \mathrm{d}\mathbf{r}$$

Lagrange Multiplier Solution

We have from the dynamical system (12) that

$$\ddot{u} + \eta\dot{u} = -\frac{\delta E}{\delta \bar{u}} - \sum_j \mu_j \frac{\delta G_j}{\delta \bar{u}} = -\delta E/\delta \bar{u} - \mu_1 \delta G_1/\delta \bar{u} = -\hat{H}u + \mu_1 u$$

that can be inserted in

$$\ddot{G}_1 + \eta\dot{G}_1 = -\int \left(\left\{ \ddot{\bar{u}} + \eta\dot{\bar{u}} \right\} u + \bar{u} \left\{ \ddot{u} + \eta\dot{u} \right\} + 2|\dot{u}|^2 \right) \mathrm{d}\mathbf{r}$$

giving an equation for the Lagrange parameter

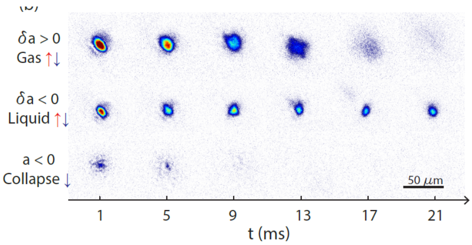
$$2E - 2\mu_1 N - 2\int |\dot{u}|^2 \mathrm{d}\mathbf{r} = -k_1 \left(1 - N\right)$$

with solution

$$\mu_1 = \frac{E + k_1 \left(1 - N\right)/2 - \int |\dot{u}|^2 \mathrm{d}\mathbf{r}}{N}$$

Note that as $\tau \to \infty$, $\mu_1 \to E$ since $|\dot{u}| \to 0$ and $N \to 1$

- The linear (usual) Schrödinger equation: $-\nabla^2\Psi_n + V(\mathbf{r})\Psi_n = E_n\Psi_n$
  - Normalized ground state: Ψ_0, $\int|\Psi_0|^2 d\mathbf{r} = 1$
  - Orthogonality, gives higher order states $\langle\Psi_n, \Psi_0\rangle = 0 \ \Rightarrow \Psi_1, \ldots$
- The non-linear Schrödinger equations (e.g.): $-\nabla^2\Psi + 2\pi\gamma|\Psi|^2\Psi + V(\mathbf{r})\Psi = \mu\Psi$
  - Ground state (mean-field) many-particle state: Ψ_0
  - Normalization: $\int|\Psi_0|^2 d\mathbf{r} = N$
  - Fixed angular momentum (rotating system): $\int\bar{\Psi}_0\hat{L}_{op}\Psi_0 d\mathbf{r} = L$
- Quantum droplets (2D): $-\nabla^2\Psi + |\Psi|^2\ln\left(|\Psi|^2\right)\Psi = \mu\Psi$



[Science, **359**, 301 (2017)]

Linear Schrödinger equation, 2D harmonic oscillator

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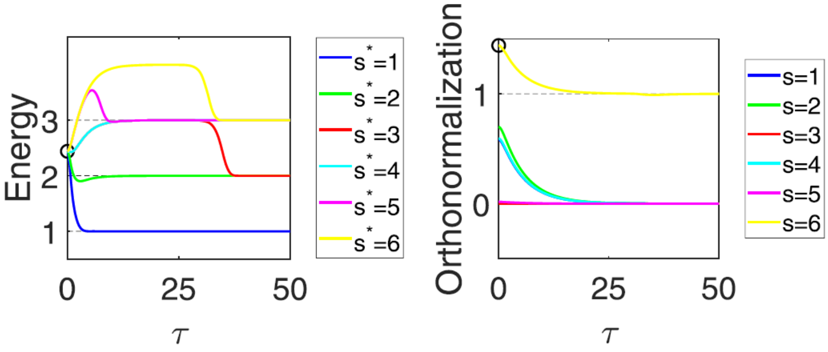


Figure 5. Left figure: Convergence of the energies for the six solutions seen in figure 4. Dashed horizontal lines correspond to the exact energies $E_{(n_x,n_y)} = n_x + n_y + 1$. Right figure: Illustration of the convergence of the calculation for solution number six (i.e. $s^* = 6$ corresponding to $n_x = n_y = 1$). The uppermost curve shows the normalization $\int |u|^2 \mathrm{d}\mathbf{r}$ (the ring shows the value $1.2^2 = 1.44$, see the initial condition in the caption of figure 4), and the lower curves show the five orthogonality constraints $\int \bar{u} u_s \mathrm{d}\mathbf{r}$, $s = 1, 2, 3, 4, 5$.

4.3. The NLSE under rotation

The NLSE is commonly used to model many interacting bosonic particles via a mean-field approximation [20]. We have developed a DFPM formulation with damped constraints for a dimensionless NLSE in $u = u(x)$ on a ring geometry $-\pi \leqslant x \leqslant \pi$ $(R = \hbar = 2M = 1)$ using periodic boundary conditions $u(-\pi) = u(\pi)$.

The aim is to minimize the total energy

$$E(u) = \int_{-\pi}^{\pi} \left|\frac{\partial u}{\partial x}\right|^2 + \pi\gamma|u|^4 \, \mathrm{d}x, \tag{34}$$

with γ a parameter for the nonlinear term, subject to one constraint for normalization, and one constraint for the angular momentum being ℓ_0

$$G_1 = 1 - \int_{-\pi}^{\pi} |u|^2 \mathrm{d}x = 0, \qquad G_2 = \ell_0 + \mathrm{i} \int_{-\pi}^{\pi} \bar{u} \frac{\partial u}{\partial x} \, \mathrm{d}x = 0. \tag{35}$$

We note that this problem can be solved analytically and refer to appendix B of reference [9] article we instead couple the minimization of equation (34) to equation (35), via the dynamical equation (13) for the constraints and get the following realization of equation (12):

$$\ddot{u} + \eta\dot{u} + \frac{\delta E}{\delta \bar{u}} + \mu\frac{\delta G_1}{\delta \bar{u}} + \Omega\frac{\delta G_2}{\delta \bar{u}} = \ddot{u} + \eta\dot{u} - \frac{\partial^2 u}{\partial x^2} + 2\pi\gamma|u|^2 u - \mu u + \mathrm{i}\Omega\frac{\partial u}{\partial x} = 0, \quad (36)$$

with the two Lagrange multipliers from equation (B.10):

$$\mu = \frac{b_1\langle\hat{\ell}^2\rangle - b_2\ell}{N\langle\hat{\ell}^2\rangle - \ell^2}, \qquad \Omega = \frac{b_2 N - b_1\ell}{N\langle\hat{\ell}^2\rangle - \ell^2}. \quad (37)$$

The Lagrange multipliers in equations (36) and (37) represent physical properties. Hence, μ is the so-called chemical potential, which is not equal to the energy E for the NLSE, and Ω is the angular velocity for the rotation. The quantities N, $\langle\hat{\ell}^2\rangle$, ℓ, b_1, b_2 in equation (37), which depend on the fictitious time τ, are defined in appendix B.

Here we consider one spatial dimension with a constraint on the angular momentum and on the interval $[-\pi, \pi]$ with periodic boundary conditions $\vec{\Psi}(-\pi) = \vec{\Psi}(\pi)$, i.e. a ring geometry. From (3) we have the energy

$$E\left(\vec{\Psi}\right) = \int_{-\pi}^{\pi} \frac{\partial \vec{\Psi}^{\dagger}}{\partial x} W \frac{\partial \vec{\Psi}}{\partial x} + \vec{\Psi}^{\dagger} V \vec{\Psi} + \pi \vec{\Psi}^{\dagger} \Gamma\left(\vec{\Psi}\right) \vec{\Psi}\, \mathrm{d}x, \tag{27}$$

and

$$\frac{\delta E(\vec{\Psi})}{\delta \vec{\Psi}^{\dagger}} = -W \frac{\partial^2 \vec{\Psi}}{\partial x^2} + V\vec{\Psi} + 2\pi\Gamma\left(\vec{\Psi}\right)\vec{\Psi}. \tag{28}$$

The constraints are

$$G_j = c_j - \int_{-\pi}^{\pi} \vec{\Psi}^{\dagger} K_j \vec{\Psi}\, \mathrm{d}x = 0, \quad j = 1, \ldots, n+1, \tag{29}$$

where

$$K_1 = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \dots & \dots & 0 \end{bmatrix}, \ldots, K_n = \begin{bmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \dots & \dots & 1 \end{bmatrix},$$
$$K_{n+1} = -i \begin{bmatrix} \frac{\partial}{\partial x} & 0 & \dots & 0 \\ 0 & \frac{\partial}{\partial x} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \dots & 0 & \frac{\partial}{\partial x} \end{bmatrix}. \tag{30}$$

5.1. Multicomponent NLSE in 1D under rotation in a ring, applications to vector solitons

In these examples we want to find normalized solutions $\vec{\Psi}(x)$ of (28) where $W = \mathrm{diag}(1, \ldots, 1)$ and $V = \mathrm{diag}(0, \ldots, 0)$, i.e.

$$\frac{\delta E(\vec{\Psi})}{\delta \vec{\Psi}^{\dagger}} = -\frac{\partial^2 \vec{\Psi}}{\partial x^2} + 2\pi\Gamma\left(\vec{\Psi}\right)\vec{\Psi} = 0, \tag{69}$$

with a constrained angular momentum.

5.1.2. Only dynamically damped constraints. From equations (29)–(31) we end up with $n+1$ dynamic constraints

$$G_j = c_j - \int_{-\pi}^{\pi} |\Psi_j|^2 \,\mathrm{d}x = 0, \;\; j = 1, \ldots, n, \quad G_{n+1} = c_{n+1} + i \sum_{j=1}^{n} \int_{-\pi}^{\pi} \overline{\Psi}_j \frac{\partial}{\partial x} \Psi_j \,\mathrm{d}x = 0. \tag{71}$$

We obtain the corresponding Lagrange parameters $\vec{\lambda}$ from the linear system given by the matrix A in (62) and the vector $\vec{b}$ in (63) by solving $A\vec{\lambda} = \vec{b}$ in each time step.

Vector non-linear Schrödinger equation, numerical results 1D

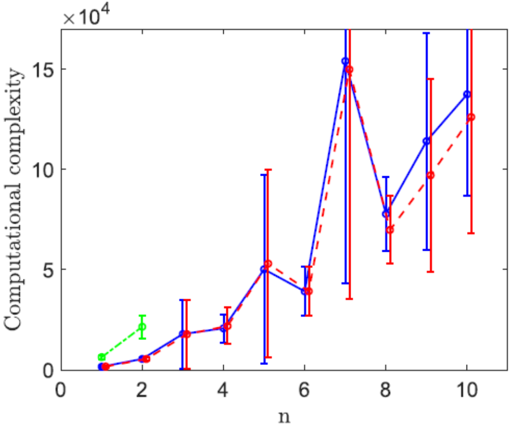
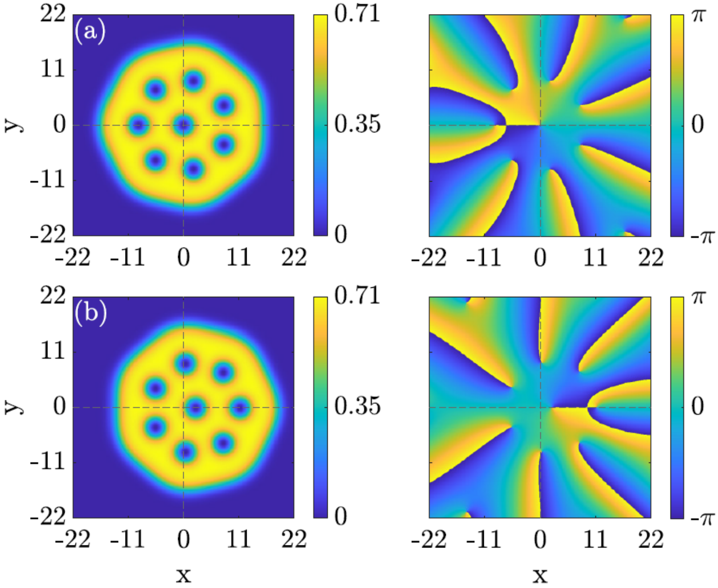
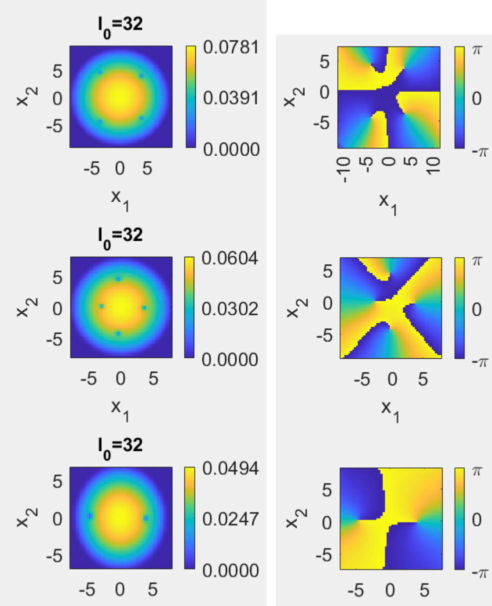


Figure 3. Benchmarking of the computational complexity for constrained n-component solutions of (69). The solid (blue) data is for *Only dynamically damped constraints* (section 5.1.2), dashed (red) data (slightly translated to the right of the integer values n for improved visibility) is for *Projection of all the normalization constraints* (section 5.1.1), dashed-dotted (green) data is for *SHAKE and RATTLE* [24] with available algorithms

Quantum Droplets, numerical results 2D



3-vector non-linear Schrödinger equation, numerical results 2D



NLSE with Manley-Rowe constraint

Normalization of a sum of functions was introduced in electrical problems by Manley-Rowe 1956.

We have implemented DFPM for a molecular-atomic pair problem where the total number of atoms are constant:

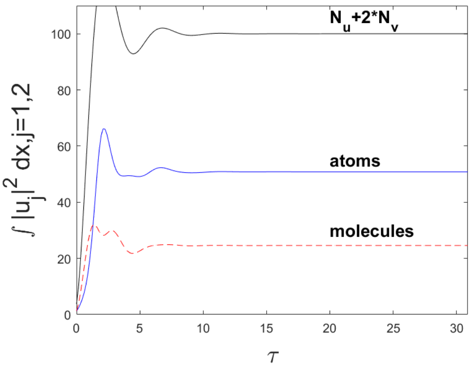
Example of only one 'mixed' normalisation constraint

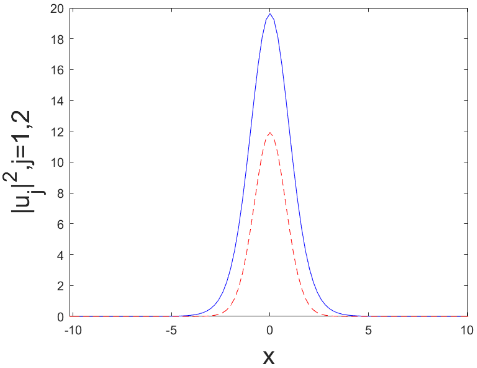
$$G_0(\Psi_1, \Psi_2) = 1 - \langle \Psi_1 | \Psi_1 \rangle - 2 \langle \Psi_2 | \Psi_2 \rangle \,.$$

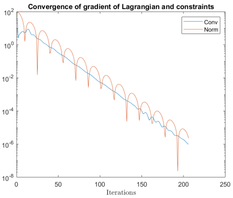
The Lagrange multiplicator can be solved for:

$$\mu_0 = \frac{k_0 G_0 - \left\langle \dot{\Psi}_1 \dot{\Psi}_1 \right\rangle - 2 \left\langle \dot{\Psi}_2 \dot{\Psi}_2 \right\rangle + \langle \Psi_1 | H_{\bar{\Psi}_1} \rangle + 2 \langle \Psi_2 | H_{\bar{\Psi}_2} \rangle}{\langle \Psi_1 | \Psi_1 \rangle + 2 \langle \Psi_2 | \Psi_2 \rangle}$$

NLSE with Manley-Rowe constraint, numerical results







Summary

The dynamical functional particle method (DFPM) with dynamical constraints

- The method is relatively insensitive to the initial conditions.
- From our experience based on the presented problems, the method performs well and is rather easy to implement.

References on developing the method for specific applications

- *The Dynamical Functional Particle Method.*
  M. Gulliksson, S. Edvardsson and A. Lind,
  https://doi.org/10.48550/arXiv.1303.5317
- *Numerical solution of the multicomponent nonlinear Schrödinger equation with a constraint on the angular momentum.*
  P. Sandin, M. Ögren and M. Gulliksson Phys. Rev. E **93**, 033301 (2016).
- *The Discrete Dynamical Functional Particle Method for Solving Constrained Optimization Problems.*
  M. Gulliksson, Dolomites Research Notes on Approximation **10**, 6 (2017).
- *Damped Dynamical Systems for Solving Equations and Optimization Problems* (2018), in Handbook of the Mathematics of the Arts and Sciences, Springer-Cham (https://link.springer.com/referenceworkentry/10.1007/978-3-319-70658-0_32-1).
- *A numerical damped oscillator approach to constrained Schrödinger equations.*
  M. Ögren and M. Gulliksson, Eur. J. Phys. **41**, (2020) 065406.
- *Dynamical representations of constrained multicomponent nonlinear Schrödinger equations in arbitrary dimensions.*
  M. Gulliksson and M. Ögren, J. Phys. A: Math. Theor. **54**, (2021) 275304.

References and future work

- Also several applications of the method done within portfolio optimization and in image analysis.

Work in progress:

- Linear Algebra Problems Solved by Using Damped Dynamical Systems on the Stiefel Manifold, e.g. new way to calculate ON-eigenstates
- Manley-Rowe constraints, e.g. the atom-molecule dynamics you saw

Dreams, to be implemented:

- Non-convex functionals...
- Excited (higher) eigenstates of non-linear functionals...

Please contact us, also after the conference, if any questions arises:
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THANK YOU!