PDE-Constrained Optimization
for Multiscale Particle Dynamics
with Industrial Applications

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Abstract

+ Later +

Contents

1 Introduction

2 DFT/ Statistical Mechanics Background

3 DDFT Background

- Some general background, link to DFT stuff

- Derivation from particle equations

- Highlight limitations of models

- Focus on overdamped equations

4 PDE-Constrained Optimization

- General Intro to the class of problems and a general problem setup

- Link to other areas?

- Literature review of Mean-Field PDECO and link between the two fields.

- Here may be a good point to go into the mean-field convergence stuf of the microscopic OCP to ours a little more.

4.1 Optimality Conditions

- Maybe here or above: discuss how to solve OCPs in different ways.

- Frechet stuff.

- Optimality conditions for the overdamped equations with Dirichlet and no-flux BCs

- Find a general notation to make future derivations 'additive'.

5 Numerical Methods

5.1 Pseudospectral Methods and 2DChebClass

- Pseudospectral Methods and Spectral Element Methods

- How shapes work

- How multishape works

- Validation in appendix??

- Convergence results for pseudospectral methods.

- Comparison with FEM and FDM

5.2 Optimization Methods

- Fixed Point (+ Armijo Extension)

- Newton-Krylov

- Picard Multiple Shooting

- fsolve Multiple Shooting

- fsolve algorithms in Matlab

6 Validation of the Numerical Methods

- Error measures

- Validation of 2DChebClass stuff

- Exact Solutions in 1D/ 2D/ (3D?!)

- Validation against fsolve (and comparison of the different solvers)

- Perturbing w

- Other things – see notes

7 Numerical Experiments

- Only examples with overdamped equations

- Maybe box and multishape?

- Paper examples (and others?)

8 Sedimentation

8.1 Background DDFT

- Derivation of the extra term from SPT, explain FMT, etc.

- A little literature review

- Comparison of simulations to Archer?

8.2 OCP

- State possible OCPs

- Derive Optimality Conditions

- Here add Periodic BCs and time-independent control

- In the future maybe also the things on curl free control

8.3 Numerical Examples

- Sedimentation examples with clustering etc in box

- Cool multishape sedimentation examples

- Comparison with overdamped result possible

- Constriction examples possible, too

- Periodic vs no-flux investigation

- Time-dependent vs time-independent control

9 Inertial Equations

9.1 Background DDFT

- Derivation of the inertial equtions from microscopic dynamics

- Limitations of the model, smoothing term for velocity

- Link to overdamped equations

- A little literature review on this type of model

9.2 OCP

- Statement of OCPs

- Derivation of optimality conditions

- Subdomain Observation, Boundary control, non-constant flux?

9.3 Numerical Examples

- 1D and 2D in box

- Comparison with overdamped model

- Some cool multishape examples?

- If subdomain and boundary stuff in this section, then those examples here too.

- Do we get in and outflow to work?

10 Multiple Species

10.1 Background DDFT

Quick literature review and illustrate coupling of equations.

10.2 OCP

- State OCP

- Derive overdamped optimality conditions

- Extend to inertial case (notation such that this is straightforward)

10.3 Numerical Examples

- Example of overdamped OCP

- Example of inertial one – comparison/agreement

- Some cool mulitshape example with two species

11 Industry application 1: Sedimentation

12 Industry application 2: Inerital multiple species

References