First Steps towards a Reduced Basis Method for Self-Consistent Field Theory Models

Alexej Disterhoft

9. September 2015

Overarching goal

We want to study the phase separation behavior of polymers.[1]

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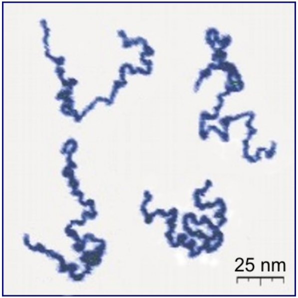
- *polymers* are large molecules, composed of many repeated subunits (*monomers*)
- monomers interact with each other in and across polymers
- theory based on stochastic models (mainly *ideal chain models*)



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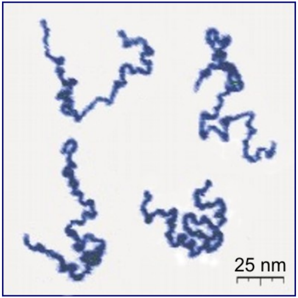
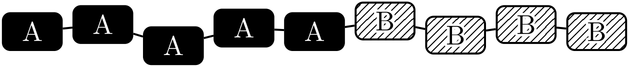
- for simplicity, we consider only *diblock copolymers*; linear chain polymers consisting of two types of monomers (e.g. A and B)





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Polymer melts (liquid phase) can exhibit different separation behaviors:

- *macrophase separation:* liquid-liquid separation (e.g. like water / oil); mostly seen in blends of different polymers.
- *microphase separation:* distinct ordering of individual polymer chains.

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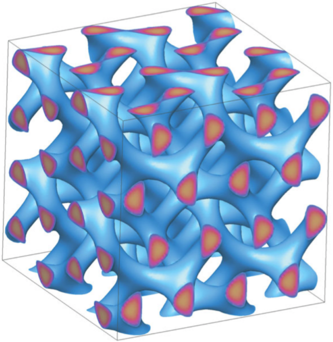
Several types of microphase separation observable depending on the properties of the polymers, e.g. gyroid.



So, what's self-consistent field theory?

Purpose of *self-consistent field theory* (SCFT):

- Goal: study a complex stochastic model (e.g. a polymer melt) with a huge number of small interacting components (e.g. monomers).
- Idea: instead of considering interactions between all the individual components, approximate the effect on a given individual by a single averaged effect (so called *external field*).

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How can this be used?

- Model leads to a free energy functional depending on external fields w_A and w_B, where *saddle points* correspond to stable microphase separations.
- Allows an iterative scheme that adjusts the external fields until these satisfy some saddle point equations.

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Most costly part of each iteration: *modified diffusion equation* (MDE)

$$\frac{\partial}{\partial s} q(\mathbf{r}, s) = c\,\Delta q(\mathbf{r}, s) - w(\mathbf{r}, s) q(\mathbf{r}, s), \quad q(\mathbf{r}, 0) = 1,$$

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where $c > 0$ and

- the normalized polymer chain contour $s \in [0, 1]$,
- a position $\mathbf{r}$ in a small volume cell $\Omega \subset \mathbb{R}^n$ (bounded domain),
- the combined external field

$$w(\mathbf{r}, s) = \begin{cases} w_A(\mathbf{r}), & 1 \leq s < f \\ w_B(\mathbf{r}), & f \leq s \leq 1 \end{cases}$$

with the ratio $f \in [0, 1]$ of A-type monomers in the polymer chain.

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Has to be solved *several hundred / thousand times* with mostly slight variations in the external fields.

Example I

- Let $\Omega = [0, 10]$ and $f = 1/2$.

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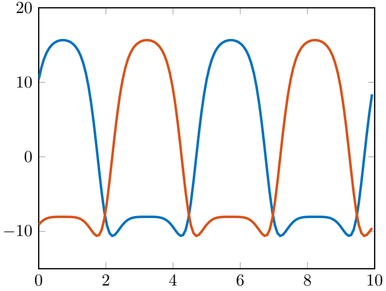

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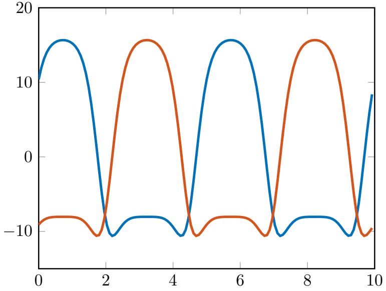
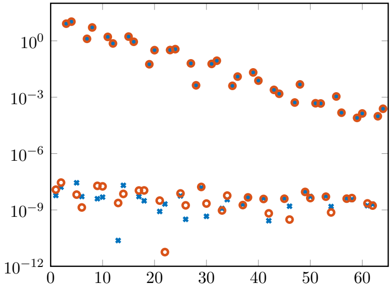
- Final fields w_A, w_B (using de facto default pseudospectral method[2]).
- Corresponding Fourier coefficients (absolute value, in the order $\cos(2\pi x), \sin(2\pi x), \cos(4\pi x), \ldots$).





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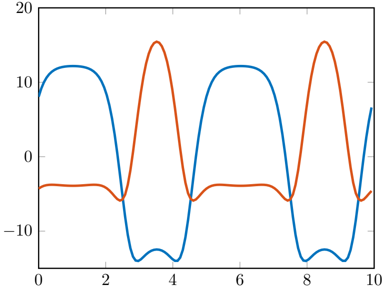
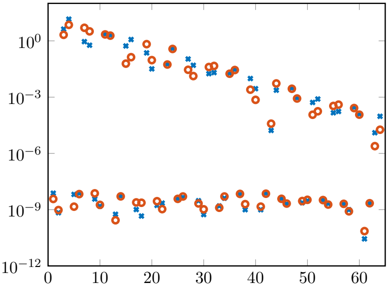
Example II

And now the same with $f = 1/3$.





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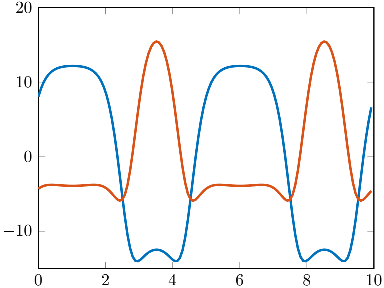

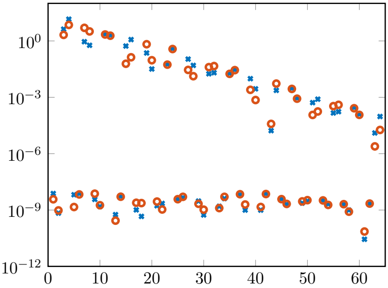

Maybe a good leverage point for model reduction by only considering the functions with significant coefficients
$\rightarrow$ model reduction by *reduced basis method*.

Intermission: Reduced Basis Method[3]

Preliminaries

Given a *parametric variational problem*

$$b(u, v; \boldsymbol{\sigma}) = f(v; \boldsymbol{\sigma}), \qquad u \in \mathcal{X},\ v \in \mathcal{Y},$$

- $\mathcal{X}, \mathcal{Y}$ are Hilbert spaces,
- $\mathcal{P} \subset \mathbb{R}^P$, $P \in \mathbb{N}$, is a closed parameter space,
- $b \colon \mathcal{X} \times \mathcal{Y} \times \mathcal{P} \to \mathbb{R}$ is a parametric continuous bilinear form,
- $f \colon \mathcal{Y} \times \mathcal{P} \to \mathbb{R}$ is a parametric continuous linear functional.

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- Assume

$$\beta(\boldsymbol{\sigma}) := \inf_{u \in \mathcal{X}} \sup_{v \in \mathcal{Y}} \frac{b(u, v; \boldsymbol{\sigma})}{\|u\|_{\mathcal{X}} \|v\|_{\mathcal{Y}}} > 0 \qquad \text{for all } \boldsymbol{\sigma} \in \mathcal{P}.$$

$+$ some minor assumptions $\Rightarrow$ for every $\boldsymbol{\sigma} \in \mathcal{P}$ exists a unique solution $u(\boldsymbol{\sigma})$.

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- Let $\mathcal{M} := \{u(\boldsymbol{\sigma}) \,|\, \boldsymbol{\sigma} \in \mathcal{P}\}$.
- Depending on the properties of the variational problem, $\mathcal{M}$ is often a *smooth manifold with low dimension*.
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Further we won't use the continuous variational problem, but instead the *truth variational problem* based on a high dimensional Galerkin method:

$$b(u, v; \boldsymbol{\sigma}) = f(v; \boldsymbol{\sigma}), \qquad u \in \mathcal{X}_{\mathcal{N}}, v \in \mathcal{Y}_{\mathcal{N}},$$

with subspaces $\mathcal{X}_{\mathcal{N}} \subset \mathcal{X}$, $\mathcal{Y}_{\mathcal{N}} \subset \mathcal{Y}$.

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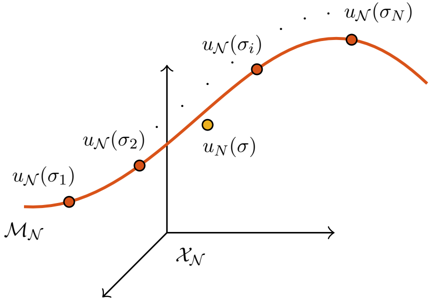
- *Offline stage:* Construction of "optimal" reduced basis spaces $\mathcal{X}_N := \{u_{\mathcal{N}}(\boldsymbol{\sigma}_n) \,|\, n = 1, \ldots, N\} \subset \mathcal{M}_{\mathcal{N}}$ and $\mathcal{Y}_N \subset \mathcal{Y}_{\mathcal{N}}$ with low dimension $N \ll \mathcal{N}$.



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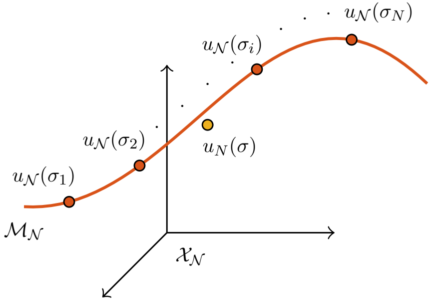
- *Online stage:* Given a parameter $\boldsymbol{\sigma} \in \mathcal{P}$, compute the rb-solution $u_N(\boldsymbol{\sigma})$ and a certified bound for the error $\|u_N(\boldsymbol{\sigma}) - u_{\mathcal{N}}(\boldsymbol{\sigma})\|_{\mathcal{X}}$ (both independent of $\mathcal{N}$).



Let $r_N : \mathcal{Y}_\mathcal{N} \times \mathcal{P} \to \mathbb{R}$ be the *residual*

$$r_N(v; \boldsymbol{\sigma}) := b(u_\mathcal{N}(\boldsymbol{\sigma}) - u_N(\boldsymbol{\sigma}), v; \boldsymbol{\sigma}) = f(v; \boldsymbol{\sigma}) - b(u_N(\boldsymbol{\sigma}), v; \boldsymbol{\sigma}).$$

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Standard theorems lead to *a posteriori error bound*

$$\|u_N(\boldsymbol{\sigma}) - u_\mathcal{N}(\boldsymbol{\sigma})\|_\mathcal{X} \leq \frac{\|r_N(\,\cdot\,;\boldsymbol{\sigma})\|_{\mathcal{Y}'_\mathcal{N}}}{\beta_{\mathrm{LB}}(\boldsymbol{\sigma})} =: \Delta_N(\boldsymbol{\sigma}),$$

where

- the norm of the residual can be efficiently computed through the Riesz representation theorem,
- $\beta_{\mathrm{LB}}(\boldsymbol{\sigma})$ is a computable lower bound for $\beta(\boldsymbol{\sigma})$.

Problem: how to compute $\beta_{\mathrm{LB}}(\boldsymbol{\sigma})$ efficiently?

[4] D. B. P. Huynh et al. "A successive constraint linear optimization method for lower bounds of parametric coercivity and inf–sup stability constants". *Comptes Rendus Mathematique* vol. 345, no. 8 (Oct. 2007), pp. 473–478. DOI: 10.1016/j.crma.2007.09.019.

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Default: *successive constraint method*[4].

- Reinterpret the calculation of $\beta(\boldsymbol{\sigma})$ as an optimization problem $\rightarrow$ linear objective function, but feasible region in general not a convex polytope.

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- Reinterpret the calculation of $\beta(\boldsymbol{\sigma})$ as an optimization problem $\rightarrow$ linear objective function, but feasible region in general not a convex polytope.
- *Offline stage:* Construct "optimal" lower and upper bounds for the feasible region.
- *Online stage:* Compute $\beta_{\mathrm{LB}}(\boldsymbol{\sigma})$ through small linear program.

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Offline stage of RBM needs a discrete "training set" $\mathcal{P}_{\text{train}} \subset \mathcal{P}$.
Iterative greedy scheme, start with random $\boldsymbol{\sigma}_1 \in \mathcal{P}_{\text{train}}$, $\mathcal{X}_1 := \{u_{\mathcal{N}}(\boldsymbol{\sigma}_1)\}$:

1. find $\boldsymbol{\sigma}_{N+1} := \arg\max_{\boldsymbol{\sigma} \in \mathcal{P}_{\text{train}}} \Delta_N(\boldsymbol{\sigma})$,
2. set $\mathcal{X}_{N+1} := \operatorname{span}(\mathcal{X}_N \cup \{u_{\mathcal{N}}(\boldsymbol{\sigma}_{N+1})\})$,
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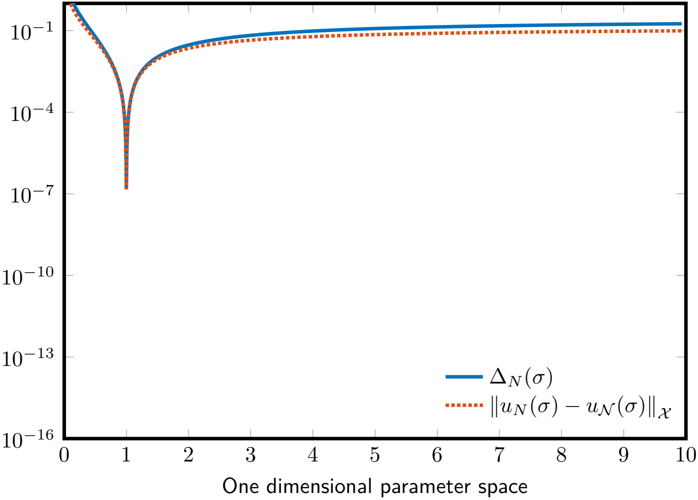
Online stage, given a $\boldsymbol{\sigma} \in \mathcal{P}$:

1. solve reduced basis system for $u_N(\boldsymbol{\sigma}) \in \mathcal{X}_N$,
2. compute certified error bound $\Delta_N(\boldsymbol{\sigma})$.

$\rightarrow$ *runtime depends only on low dimension N, not $\mathcal{N}$*.

Typical results of the offline stage, one dimensional parameter space.



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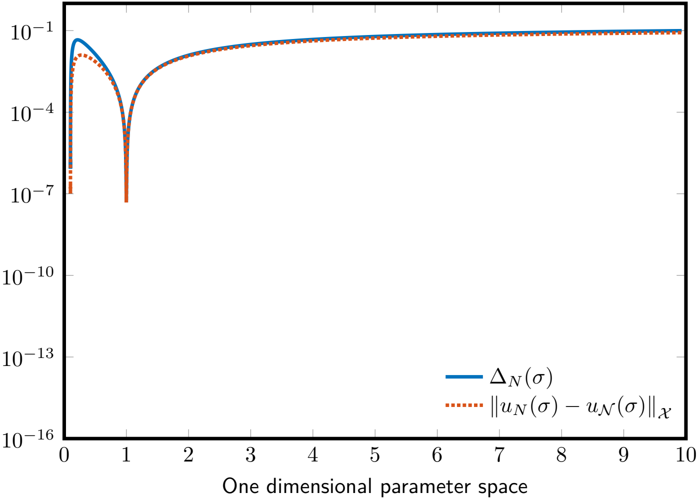

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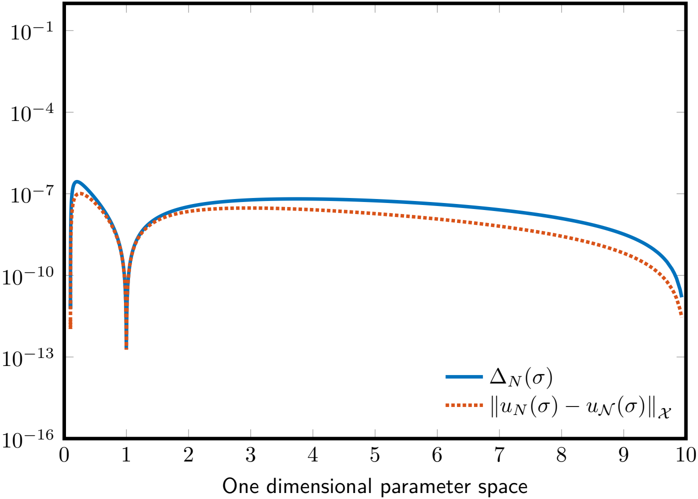

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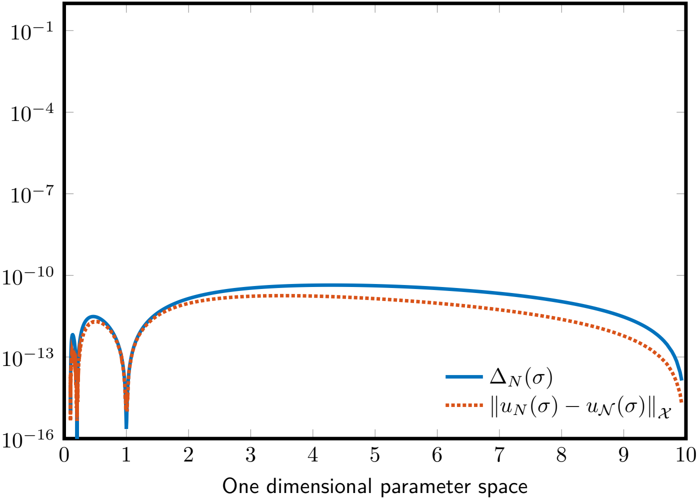
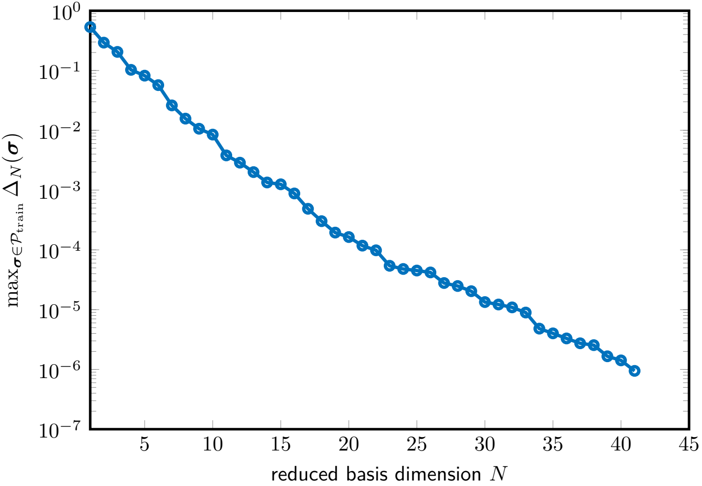


And now a four dimensional parameter space.



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  where $N \in \mathbb{N} \cup \{\infty\}$, $\boldsymbol{\sigma} \in [-1,1]^N$ and $\phi_j \in L_\infty(\Omega)$, $j = 1, \dots, N$.
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- Shown that the solution of the STVP depends *analytically* on the parameters (given some restrictive sufficient conditions).
- Applied a *Petrov-Galerkin* method to solve the STVP.
- Experimented with the application of the reduced basis method on the STVP.

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Problems encountered so far:

- The fact that $\mathcal{X} \neq \mathcal{Y}$ complicates lots of things.
- Most suitable Petrov-Galerkin methods aren't unconditionally stable.
- Successive constraint method suffers from curse of dimensionality and is quite slow for more than a handful of parameters.
  $\rightarrow$ a priori knowledge about field expansion functions required to reduce number of parameters.