Application of Model Reduction to Modelling and Simulation of Microfluidic Systems

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16th December 2008

Outline

Microfluidic devices

- First microfluidic devices appeared in the late of 1980s and rapid progress in microfluidics was made in 1990s.
- The majority of its applications in life science and medical treatment were medical diagnostic, genetic sequencing, drug discovery and proteomics.
- To analyse liquids, one forces them to flow through microchannels.

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Treating fluids in small-scale

Molecules

Treating fluid as a collection of individual, interactive molecules.

Continuum

Considering fluid as matter that is defined everywhere (continuum).

The latter is chosen.

- Simpler since using existing results for the "medium-scale" flows.
- Some flows can be computed analytically.

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Mathematical Model of Flows

Navier-Stokes equations are utilized [12]. Spatial discretization of such equations leads to

First-order system

$$Ex'(t) = Ax(t) + Bu(t),$$
$$y(t) = Cx(t);$$

Second-order system

$$Mx''(t) + Dx'(t) + Kx(t) = Qu(t),$$
$$y(t) = Lx(t).$$

Definition

The dimension of $x(t)$ is called the size of the system.

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The dimension of $x(t)$ is called the size of the system.

Why MR has to be utilized?

Size of system is typically very large, depends on

- Required accuracy;
- Geometric complexity.

UP TO $10^5, 10^6$

- Computers can not handle such large data;
- Take much time to compute.

Problem

How to replace a large system by a much smaller system which retains the essential properties?

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Balanced Truncation

details

- First proposed by B. C. Moore (1981) for first-order systems [17];
- Only for small, medium systems
- Giving global error bound and preserving stability;
- Developed for second-order systems by , e.g. Y. Chahlaoui (2006) *et al* [4], C. Hartmann (2008) *et al* [13].....

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- Interpolating the transfer function around some point s_0 by matching some first coefficients of Taylor's expansion about s_0;
- Suitable for large systems;
- No global error bound [1, 2];
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$\mathcal{H}_2$-Optimal based model reduction

- Optimizing the $\mathcal{H}_2$-norm error functional between the original transfer function and the reduced one:

$$min\|H - H_r\|^2_{\mathcal{H}_2}$$

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Some other methods

- Multipoint moments matching;
- Tangential interpolation;
- Quasi-convex optimization;
- Hybrid method...

Example

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Heat equation $\rho C_\rho \frac{\partial T}{\partial t} - \nabla(\kappa \nabla T) = Q$, on Ω; boundary condition $(\frac{\partial T}{\partial n} + k_i T)|_{\partial \Omega_i} = 0$, $\cup_{i=1}^{N} \partial \Omega_i = \partial \Omega$. Spatial discretization leads to the system

$$Ex'(t) + (A_0 + \sum_{i=1}^{N} k_i A_i)x(t) = Bu(t),$$
$$y(t) = Cx(t).$$

Why Parametric Model Reduction???

Facts

- Conventional method only applied when the values of k_i are fixed;
- k_i change, model reduction must be performed from the beginning;
- Simulation the same model but different values of parameters;

Demand

Reducing the model and symbolically preserving the parameters

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Situation in Modelling Microfluidic Systems

Example

When reducing the systems formed by discretization of dimensionless version of Navier-Stokes equations, one also has to take into consideration some parameters

- Reynolds number;
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Problem Statement

Given a parameters-dependent systems of size N

$$M(p)x''(t) + D(p)x'(t) + K(p)x(t) = Qu(t),$$
$$y(t) = Lx(t), p = (p_1, ..., p_k).$$

Replace it with a parameters-dependent systems of size $n, n << N$

$$M_n(p)x''(t) + D_n(p)x'(t) + K_n(p)x(t) = Q_n u(t),$$
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Existing Results

- Some authors: L. Daniel *et al*(2004) [5], L. H. Feng *et al* (2005) [7, 8], C. Moosmann (2007) [19];
- All approaches are based on multivariable expansion of transfer function and matching the "generalized moments";
- Projecting matrices are constructed via Krylov subspace;
- Rapid increase of mixed moments and storage of huge data need further investigation;

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Goal of thesis is to develop parametric model reduction method and apply the result to modelling and simulation of microfluidic systems.

Outline

- Improvement of the existing approaches: construction of projecting matrices, implementation algorithms,...
- Parametric model reduction for second-order systems;
- Novel methods.

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End

THANK YOU!

For an observable, reachable and stable system with $E = I$, infinite gramians:

$$\mathcal{P} = \int_0^\infty e^{A\tau} B B^T e^{A^T\tau} d\tau, \quad \mathcal{Q} = \int_0^\infty e^{A^T\tau} C^T C e^{A\tau} d\tau$$

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The balancing transformation T: back

$$\tilde{\mathcal{P}} = \tilde{\mathcal{Q}} = \Sigma = diag(\sigma_1, ..., \sigma_k, ..., \sigma_n)$$

Does it exist?

Theorem

For an observable, reachable and stable system, there exists a balancing transformation

$$T = \Sigma^{1/2} K^T U^{-1}, T^{-1} = UK\Sigma^{-1/2},$$

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Transfer function

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\begin{aligned}
H(s) =& C(sE - A)^{-1}B \\
=& -C((s - s_0)E - (A - s_0E))^{-1}B \\
=& -C(I - (s - s_0)(A - s_0E)^{-1}E)^{-1}(A - s_0E)^{-1}B \\
=& -C\sum_{i=0}^{\infty}((A - s_0E)^{-1}E)^i(A - s_0E)^{-1}B(s - s_0)^i \\
=& \sum_{i=0}^{\infty} M_i(s - s_0)^i.
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$\mathcal{K}_m(A, B) = \text{span}\{B\ AB\ A^2B\ ...A^{m-1}B\}.$

$\mathcal{K}_{i+1}(((A - s_0E)^{-1}E)^T, C^T), \mathcal{K}_{i+1}(((A - s_0E)^{-1}E), (A - s_0E)^{-1}B).$

$\text{span}\, W = \mathcal{K}_{i+1}(((A - s_0E)^{-1}E)^T, C^T)$
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