MATMOL: a MATlab Method Of Lines library

Description

Many physical and chemical processes are distributed parameter systems, i.e., systems in which state variables depend on several independent variables (such as time and space), and which are described by sets of nonlinear partial differential equations (PDEs). The method of lines (MOL) is probably the most widely used approach to the solution of evolutionary PDEs, and the objective of this paper is to report on the development of a Matlab© based MOL toolbox.

Basically, the MOL proceeds in two separate steps:

- approximation of the spatial operators, using finite difference, finite element, finite volume methods, and
- time integration of the resulting semi-discrete (discrete in space and continuous in time) equations using an ODE or DAE solver.

MATMOL contains a set of linear spatial approximation techniques, e.g., finite difference methods, implemented using the concept of differentiation matrices, as well as a set of nonlinear spatial approximations, e.g., flux limiters. In addition, several time integrators, including basic explicit methods and some advanced linearly implicit methods, are included.
In this new version of the MATMOL two new functions are included. The first one (`mfem_fselib.m`) was constructed from the FSELIB (5) and allows the user to compute the numerical solution of 1D PDE systems using the Finite Element Method (FEM) (3). The second one (`pod_computation.m`) is employed for computing the basis functions which allow the projection of the system dynamics into a low dimensional subspace thus reducing the number of equations of classical techniques such as FEM or FD. For more information about this technique, the reader is referred to the bibliography (1; 2; 7; 6).
A more detailed description about the use of these new functions is included in the user's manual of the `mfem_fselib` function (see `user_manual_fselib.pdf`).

Philosophy

The underlying philosophy of these developments is to provide the user with a variety of easily understood methods, and a collection of application examples that can be used as Matlab© templates for the rapid prototyping of new dynamic simulation codes.

The MATMOL is available free of charge FOR NON-COMMERCIAL use on an as is basis. The authors cannot be held liable for any deficiency, fault or inconvenience resulting from the use of MATMOL.

Version history and contents

2004: Version: 1.0

- 1D and 2D finite difference and finite volume approximation stencils on uniform and nonuniform grids.
- Examples: Burgers' equation and a catalytic reactor.
- Reference: (4)

2008: Version: 1.1

- Addition of advanced nonlinear solution techniques: flux limiting functions and adaptive gridding techniques.
- Additional examples: a dispersive jacketed tubular reactor (to be downloaded separately).
- Reference: (8)

2009: Version: 1.2

- Addition of the FEM in 1D problems.
- Addition of the POD technique for model reduction.

Installation

The `matmol.zip` file containing the MATMOL package is available upon request (by emailing one of the authors) or can be downloaded from the website of the Service d'Automatique of the Faculté polytechnique de Mons[1] under the section `Research - Distributed parameter systems`. The installation is easy and proceeds in the following steps:

1. Unzip the zip file to a desired directory, e.g., `C:/Program Files/MATLAB/R2006a/MATMOL`
   Seven subdirectories are unzipped:
   - `Dynamic_Regridding`, containing the dynamic regridding files,
   - `FD_non_uniform_grids`, containing the finite difference stencils on nonuniform grids,
   - `non_uniform_grids`, containing the finite difference stencils on uniform grids,
   - `Slope_limiters`, containing the flux limiting files,
   - `Static_Regridding`, containing the dynamic regridding files,

[1] `http://www.autom.fpms.ac.be/index_english.html`

- `Slope_limiters`, containing the flux limiting files, and
- `pdes`, containing the template files for the examples of Burgers' equation and a catalytic reactor.
- `FEM_POD`, containing the files for the FEM and the POD techniques.

2. Add all seven subdirectories to your Matlab© path to make then accessible from any directory.

3. Try your configuration by running `burgers_main.m`.

Updates

Updates and novel developments are announced on the website of the Service d'Automatique of the Faculté polytechnique de Mons. Alternatively, by sending an e-mail to Alain Vande Wouwer `Alain.VandeWouwer@fpms.ac.be` it is possible to join the MATMOL mailinglist which informs about updates and new features.

Bibliography

[1] L. Sirovich. Turbulence and the dynamics of coherent structures. Part I: Coherent structures. *Quaterly of Appl. Math.*, 45(3):561–571, 1987.

[2] G. Berkooz, P. Holmes, and L. Lumley. The Proper Orthogonal Decomposition in the analysis of turbulent flows. *Ann. Rev. Fluid Mech.*, 25:539–575, 1993.

[3] J. N. Reddy. *An Introduction to the Finite Element Method*. McGraw-Hill, 2nd edition, 1993.

[4] A. Vande Wouwer, P. Saucez, and W.E. Schiesser 2004. Simulation of distributed parameter systems using a Matlab-based method of lines toolbox: Chemical engineering applications, *Industrial and Engineering Chemistry Research*, 43, 3469-3477.

[5] C. Pozrikidis. *Introduction to Finite and Spectral Element Methods using Matlab*. Chapman & Hall/CRC, 2005.

[6] M. R. García. *Identification and Real Time Optimisation in the Food Processing and Biotechnology Industries.* PhD thesis, University of Vigo, Spain, May 2008. Available online at http://digital.csic.es/handle/10261/4662.

[7] C. Vilas. *Modelling, Simulation and Robust Control of Distributed Processes: Application to Chemical and Biological Systems*. PhD thesis, University of Vigo, Spain, May 2008. Available online at http://digital.csic.es/handle/10261/4236.

[8] F. Logist, P. Saucez, J.F. Van Impe, and A. Vande Wouwer 2009. Simulation of 1D reaction-diffusion-convection processes using Matlab: comparison and guidelines. *(submitted)*