# MATMOL: a MATlab Method Of Lines library

The MATMOL Group (2009)

# 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<sup>©</sup> 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 version of the MATMOL new approaches are included:

- A 1D version of the finite element method (FEM) constructed from the FSELIB library (4). See the matfem function user's manual for details.
- Spectral methods like the laplacian spectral decomposition (LSD), the proper orthogonal decompositions (POD) or the Chevichev polynomials. See the matlsd and matpod function user's manuals for details.

For more information about these techniques, the reader is referred to the bibliography (6; 1; 8; 2; 5; 9).

## 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<sup>©</sup> 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: (7)

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: (3)

2009: Version: 1.2

- Addition of the FEM in 1D problems.
- Addition of spectral methods like the laplacian spectral decomposition, the POD technique for model reduction and Chevichev polynomials.

### Installation

The different files containing the MATMOL packages can be FREELY downloaded from the webpage <u>www.matmol.org</u>. A free registration is required before downloading the packages. In the menu at the left of the screen you will find the label Methods and inside it four different options:

- Linear\_operators, containing a zip file with the finite differences files (including dynamic and static regridding and for both, uniform and non uniform grids), the finite element method and other spectral techniques like the proper orthogonal decomposition, the laplacian spectral decomposition or Chevichev polynomials.
- Nonlinear\_operators, containing a zip file with the flux limiting codes.
- Hybrid, containing a zip file with the splitting methods. It should be mentioned that, in this case, the method is in the form of a template example (DFR\_Seq\_Meth) since this technique is problem dependent.
- All together, containing a zip file with all the codes of the MATMOL.

The installation is easy and proceeds in the following steps:

- 1. Choose one of the proposed methods (or alternatively all together) and download the corresponding zip file.
- 2. Unzip the zip file to a desired directory, e.g., C:/Program Files/MATLAB/ R2006a/MATMOL. A number of subdirectories, which will depend on the chosen method, are unzipped.
- 3. Add all new subdirectories to your Matlab<sup>©</sup> path to make then accessible from any directory.

In order to try the configuration and for illustrative purposes, a number of examples (including some benchmark problems) are available in the MATMOL webpage (see the Examples section). The structure of this section is practically the same as in the case of Methods. The only difference is that the Hybrid folder is not included since the examples in this case were already included in the Methods section. The user is recommended to read the Benchmark examples document (also included in the MATMOL webpage) for more information.

- Download the zip files containing the examples you desire to test
- Unzip them into a given directory.
- Try the test by running the main file, e.g., burgers\_main.m.

## Updates

Updates and novel developments are announced on the website of the MATMOL toolbox. 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.

#### References

- [1] 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.
- [2] 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.
- [3] 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*)
- [4] C. Pozrikidis. *Introduction to Finite and Spectral Element Methods using Matlab*. Chapman & Hall/CRC, 2005.
- [5] J. N. Reddy. *An Introduction to the Finite Element Method*. McGraw-Hill, 2nd edition, 1993.
- [6] L. Sirovich. Turbulence and the dynamics of coherent structures. Part I: Coherent structures. *Quaterly of Appl. Math.*, 45(3):561–571, 1987.
- [7] 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.
- [8] 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.
- [9] O. C. Zienkiewicz, R. L. Taylor, and J. Z. Zhu. *The Finite Element Method: Its Basis & Fundamentals.* Elsevier, Amsterdam, 6<sup>th</sup> edition, 2005.