295 Mathcad[1] Worksheets for Ordinary Differential Equations

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Abstract

The purpose of the paper is to introduce a set of Mathcad worksheets containing systems of ordinary differential (ODE) equations. They can be used to become familiar with the Mathcad implementation of differential equations and with the behavior of dynamical systems in general. The problems are taken from a collection of test examples for data fitting in dynamical systems, see Schittkowski [78]. The report contains a summary of 295 differential equations that have been transferred to Mathcad and a detailed example. All worksheets can be downloaded from the home page of the author[2]. A particular advantage of executing these problems from Mathcad is the possibility to plot corresponding solutions very easily.

[2]http://www.klaus-schittkowski.de

1 Introduction

We consider systems of ordinary differential equations with initial values given in the form

$$
\begin{aligned}
\dot{y}_1 &= F_1(y,t) \ , \quad y_1(0) = y_1^0 \ , \\
&\cdots \\
\dot{y}_n &= F_n(y,t) \ , \quad y_s(0) = y_n^0 \ .
\end{aligned}
\tag{1}
$$

Without loss of generality, we allow that the initial time is zero, as in many real-life situations. At $t = 0$, initial values of the differential equations are y_1^0, ..., y_n^0. The solution depends on the time variable t and is denoted by $y(t)$. It is assumed that the right-hand side of (1) is defined by a continuous function $F(y,t) = (F_1(y,t), \ldots, F_n(y,t))^T$.

Example 1.1 *A very simple system of two linear differential equations, which could describe a kinetic biological or chemical process, is given by*

$$
\begin{aligned}
\dot{y}_1 &= -k_1 y_1 \ , & y_1(0) = D \ , \\
\dot{y}_2 &= k_1 y_1 - k_2 y_2 \ , & y_2(0) = 0 \ ,
\end{aligned}
$$

where reaction coefficients k_{12}, k_{21} and an initial dose D are given. In this particular case, the solution is known explicitly and is given by

$$
\begin{aligned}
y_1(t) &= D\, e^{-k_1 t} \ , \\
y_2(t) &= \frac{k_1 D}{k_1 - k_2} \left(e^{-k_2 t} - e^{-k_1 t} \right) \ .
\end{aligned}
$$

as can be proved by insertion.

The software system EASY-FIT, see Schittkowski [78], comes with a collection of 1,000 test examples for data fitting in dynamical systems. Among them are 463 systems of ordinary differential equations, where some parameters of the right-hand side or the initial conditions are to be fitted. Most problems have some practical background.

However, the basic structure of these problems is more general and adopted to data fitting. For example, some of the test problems possess additional constraints, there are break or switching points where the system changes its structure, and some of the data fitting test problems only differ in the data, not the dynamical system. Moreover, some of the problems are too complex for the purpose of this collection. Thus, a subset of 295 test problems is selected and re-implemented in Mathcad. The mcd-files can be downloaded from the home page of the author,

`http://www.uni-bayreuth.de/departments/math/~kschittkowski/home.htm`

The report is one out of a series of Mathcad test problem collections by which numerical routines are tested and the implementation of optimization problems and dynamical systems is outlined, i.e.,

1. nonlinear programming [80],
2. data fitting [81],
3. differential algebraic equations [82],
4. partial differential equations [83],
5. partial differential algebraic equations [84].

Section 2 contains a brief outline of the implicit integration routine called *Radau* in Mathcad, which is used for all test cases. A simple example is shown in Section 3 to illustrate the numerical solution of differential equations. A list of the Mathcad worksheet files and some further details about problem structure, background, and source is given in Section 4.

2 Implicit Solution Methods

A characteristic property of explicit integration methods for differential equations is that a new approximation of the solution is evaluated explicitly from the known one at a previous time, and from some intermediate function values of the right-hand side of the ODE. This iterative integration process breaks down in case of numerical instability of the underlying differential equation. One possible reason is the existence of large and small eigenvalues of the Jacobian of the right-hand side $F(y,t)$ of (1). In these situations, we say that the differential equation is *stiff* and we need more powerful, that are more stable, ODE solvers.

Implicit methods are defined by a full Butcher array or tableau, respectively, and possess excellent stability properties. Let h_j be a stepsize of the j-th integration step, $t_{j+1} = t_j + h_j$ a new trial point with $t_0 = 0$, and η_j a known approximation of the solution $y(t_j)$ starting from $\eta_0 = y_0$. Then a new approximation η_{j+1} is obtained from

$$\eta_{j+1} = \eta_j + h_j \sum_{i=1}^{r} b_i k_i \quad , \tag{2}$$

where the coefficients k_i depend on η_j and are obtained by solving a system of rs nonlinear equations

$$k_i = F(\eta_j + h_j \sum_{m=1}^{r} a_{im} k_m, t_j + h_j c_i) \tag{3}$$

for $i = 1, \ldots, r$. Note that each k_i is n-dimensional, where n denotes the number of differential equations in (1). The numerical integration starts at $t = 0$ and stops as soon as a given time value t is reached. The choice of the stage number r and the coefficients a_{im} and b_i depends on the desired stability and order conditions. The coefficients c_i are usually chosen so that

$$c_i = a_{i1} + \cdots + a_{i,r}$$

for $i = 1, \ldots, r$.

If $a_{im} = 0$ for all $i \leq m$, we get an explicit integration method, for example a Runge-Kutta method. In case of $a_{im} = 0$ for all $i < m$ and $a_{ii} \neq 0$ for at least one i, we get a diagonal implicit Runge-Kutta method. Moreover, if all diagonal elements a_{ii} are constant and different from zero, we say that the method is singly diagonal implicit. For the numerical tests reported in this report, we use a fully implicit method of the Radau type with three stages and order 5 (RADAU5) as described in Hairer and Wanner [35].

The computational work of an implicit method increases drastically compared with an explicit method. For each integration step j, we have to solve a system of rs nonlinear equations, where usually Newton's method is applied. Thus, implicit ODE methods need the Jacobian of the right-hand side $F(y,t)$ either in analytical form or computed by internal numerical approximation. Whenever possible, special structures of the Jacobian are exploited, for example a band structure. One can also try to use Jacobian matrices from previous iterations whenever it seems to be profitable.

To give an example, we consider Runge-Kutta-type methods based on so-called Radau and Lobatto quadrature formulae, see Butcher [16] or Hairer and Wanner [35]. A frequently used variant is the implicit Runge-Kutta method of type Radau IIA, a simple integration method of order 3 with two stages defined by the tableau

$$\begin{array}{c|cc} \frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

The implicitly given formulae to compute the coefficients k_i are

$$\begin{aligned} k_1 &= F(\eta_j + h_j(5k_1 - k_2)/12, t_j + h_j/3) \ , \\ k_2 &= F(\eta_j + h_j(3k_1 + k_2)/4, t_j + h_j) \ , \end{aligned}$$

and an approximation of the solution is

$$\eta_{j+1} = \eta_j + h_j(3k_1 + k_2)/4 \ .$$

A more advanced implicit Runge-Kutta formula of type Radau IIA is obtained from the array

$$\begin{array}{c|ccc}
\frac{4-\sqrt{6}}{10} & \frac{88-7\sqrt{6}}{360} & \frac{296-169\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{225} \\
\frac{4+\sqrt{6}}{10} & \frac{296+169\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} \\
1 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \\
\hline
 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9}
\end{array} \tag{4}$$

The implicit method possesses three stages and is of order 5, see Hairer and Wanner [35].

3 A Mathcad Worksheet Example

Mathcad (`http://www.mathcad.com`) is an interactive GUI with a large number of built-in mathematical functions. Special commands allow to solve systems of ordinary differential equations, especially also stiff equations by the implicit Radau method introduced in the previous section. The subsequent lines describe the usage of *Radau*, see also the Mathcad documentation
A call of *Radau(y, x1, x2, npoints, D)* returns a matrix in which the first column contains the points at which the solution to the ODE is evaluated and the remaining columns contain the corresponding values of the solution and its first $n-1$ derivatives.

Arguments:

- y must be either a vector of n initial values or a single initial value.
- *x1, x2* are endpoints of the interval on which the solution to differential equations will be evaluated. Initial values in y are the values at *x1*.
- *npoints* is the number of points beyond the initial point at which the solution is to be approximated. This controls the number of rows *1 + npoints* in the matrix returned by Radau.
- D is an n-element vector-valued function containing the first derivatives of the unknown functions, i.e., the right-hand side of the differential equation.

To give an impression how a test problem is implemented, we consider problem LKIN, a simple linear kinetic process outlined in Example 1.1.

LKIN

Ordinary Differential Equation

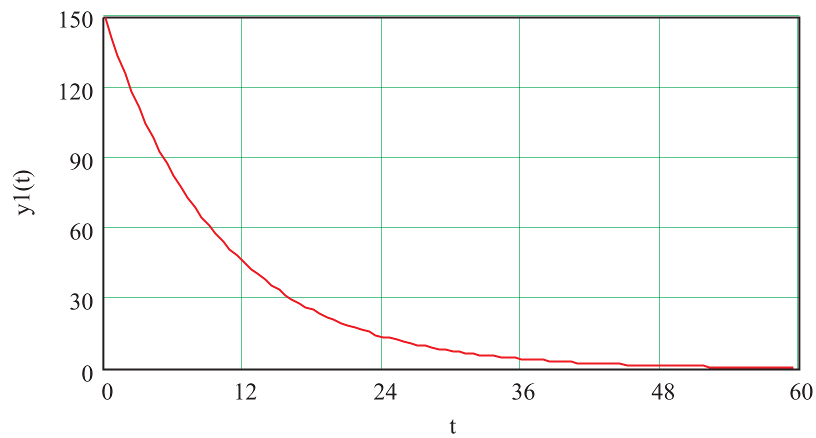
Description: Simple linear compartment model

Constants: $k1 := 0.1 \quad k2 := 0.05 \quad D := 150$

Initial Values: $y := \begin{pmatrix} D \\ 0 \end{pmatrix} \quad \begin{pmatrix} y1 \\ y2 \end{pmatrix}$

Differential Equation: $D(t, y) := \begin{pmatrix} -k1 \cdot y_1 \\ k1 \cdot y_1 - k2 \cdot y_2 \end{pmatrix}$

Integration: $Y := \text{Radau}(y, 0, 60, 100, D)$



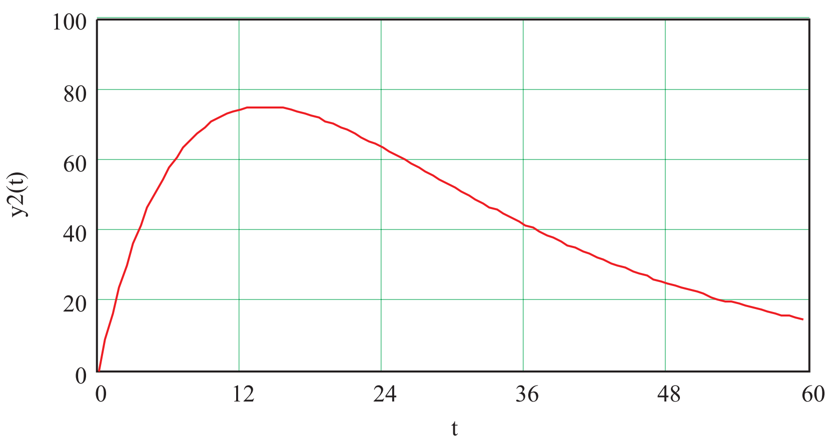


Figure 1: Mathcad Implementation

4 List of All Test Problems

The subsequent table contains a list of all test problems together with the number of equations n, a brief description of the practical or mathematical background, and some references. The differential equations have first been implemented in the modelling language PCOMP, see Dobmann et al. [20] or Schittkowski [78, 77, 79]. The transformation into Mathcad worksheets follows a unified format based on the PCOMP equations. Thus, the implementations do not exploit all possible features of Mathcad to get the most elegant and compact description. All mcd-files can be downloaded from the home page of the author[3].

Table Ordinary Differential Equations

name	n	*background*	*ref*
2LNK_ROB	4	Two-link planar robot without constraints	[3]
2ND_ORD	2	Academic test problem, ill-behaved second order IVP	[15], [96]
2ND_RATE	1	Second order rate equation under heat transfer conditions	[102]
ACTIVITY	2	Activities over time	
ACTNITR	8	Nitrification in activated sludge process	[21]
ADIABATI	2	Adiabatic complex gas-phase reaction in a PFR	[102]
AEKIN	3	AE-kinetics	
AIRY	2	Airy equation	[95]
AKTIV_W2	4	Association kinetics, two-state-theory	
ALPHA_PI	5	Isomerization of an alpha-pinene	
AMIDPRO	4	Amidproton replacement with protein folding	
AMMONAB	3	Steady-state absorption column design	[40]
AMYLASE	7	Alpha-amylase production with bacillus subtilis	
ANAEMEAS	7	Anaerobic reactor activity	[21]
ANHYD	3	Oxidation of o-xylene to phthalic anhydride	[40]
ANTIBIO	2	Kinetics of antibiotics in liquid manure	[70]
APPRX1	1	Curve fitting	[106]
APPRX2	1	Curve fitting	[106]
ASS_CV1	7	Association curves	
ASS_CV2	2	Association curves	
ASS_CV3	2	Association curves	

(continued)

[3] http://www.klaus-schittkowski.de

name	*n*	*background*	*ref*
ASS_CV4	2	Association curves	
ASS_CV5	3	Association curves	
ASS_CV6	3	Association curves	
ASS_CV7	2	Association curves	
ASS_KIN1	1	Association kinetics	
ASS_KIN2	1	Association kinetics with exponential term	
ASS_KIN3	1	Association kinetics	
ASS_KIN4	1	Association kinetics	
ASS_KIN5	2	Association kinetics	
ASTRO	4	Planar motion of earth around sun (singularities)	[3]
ASYMP	2	Asymptotic boundary value problem	[3]
AXDISP	16	Differential extraction column with axial dispersion	[40]
BARN1	2	Chemical reaction, Lotka-Volterra equation	[98]
BARN2	2	Chemical reaction, Lotka-Volterra equation with variable initial values	[98]
BATCHD	1	Dimensionless kinetics in a batch reactor	[40]
BATCOM	4	Batch reactor with complex reaction sequence	[40]
BATEX	2	Single solute batch extraction	[40]
BATFERM	3	Batch fermentation	[21]
BATSEG	2	Simple reaction with segregation in a batch reactor	[40]
BATSEQ	4	Complex batch reaction sequence	[40]
BEAD	6	Diffusion and reaction in a spherical bead	[40]
BEER	7	Beer fermentation	
BELLMAN	1	Chemical reaction (Bellman)	[99]
BELUSOV	4	Oscillating chemical reaction, highly stiff (Belusov-Zhabitinsky)	
BENZENE	2	Pyrolytic dehydrogenation of benzene to diphenyl	
BENZHYD	2	Isothermal tubular reactor with two consecutive reactions (dehydrogenation of benzene)	[40]
BI_OSC	2	Chaotic bi-stable oscillator	[12], [33]
BIMOLECU	1	Carcino-embryonic antigen binding, bimolecular reversible reaction	[1]
BIODEG	3	Degradation of two substrates and growth of biomass	
BIOPROC	3	Recombinant microbiological process	[23]
BLOOD_O	1	Blood ethanol concentration	[99]
BRUNHILD	3	Bolus injection of radioactive sulfate	[88]
BRUSSEL1	6	Multi-molecular reaction (Brusselator)	[50]
BRUSSEL2	2	Multi-molecular reaction (Brusselator)	[34]

(continued)

name	*n*	*background*	*ref*
BSTILL	11	Binary batch distillation column (nine floors)	[40]
BVP	2	Boundary value problem	[3]
BVP4	16	Complex 4-th order boundary value problem (normal mode decomposition of PDE)	
CABBAGE	3	Growth of white cabbage (roots, stem, leaves)	[70]
CARGO	6	Transferring containers from ship to truck	[25], [97]
CASC_IMP	11	Air humidity in laboratory device	
CASCADE1	5	Storage cascade of flow in pipes, Riccati equation	[51]
CASCADE2	1	Flow in pipes with one storage, Riccati-Muskingum equation	[51]
CASCSEQ	12	Cascade of three reactors with sequential reactions	[40]
CASTOR	2	Batch decomposition of acetylated castor oil	[40]
CAT_HYD	2	Catalytic hydrolysis of acetic anhydride	[100]
CHAIN_O1	2	First-order reversible chain reaction	[98]
CHAN_FLO	4	Flow of a fluid during injection into a long channel	[19]
CHANNEL	3	Flow in a channel (3rd order BVP)	[3]
CHEM_OSC	5	Chemical oscillator	[38], [89]
CHEM_REA	9	Chemical reaction	
CHEMO	3	Chemostat fermentation	[21]
CIRCLE	4	Parameterized circle equation	
COLCON	11	Extraction cascade with backmixing and control	[40]
COLLISIO	8	Collision dynamics between an Argon and a Neon atom in their mutual Lennard-Jones force field	[85]
COMMENSA	7	Two bacteria with opposite substrate preferences	[21]
COMP_EXP	2	Two compartments with equal absorption and exponential elimination	[68]
COMPASM	5	Competitive assimilation and commensalism	[21]
COMPET	2	Competition of two species	[12], [5]
COMPREAC	7	Complex reaction scheme between formaldehyde and sodium para phenol sulphonate	[40]
COMPSEG	6	Complex reaction with segregation in a semi-batch reactor	[40]
CON_BURG	2	Burgers' equation with state and boundary constraints	[8]
CONC4	1	Chemical simulation model	
CONF_ALT	2	Conformation alterations of proteins	
CONFLO1	1	Continuous open tank flow	[40]
CONINHIB	2	Continuous culture with inhibitory substrate	[21]
CONSTILL	10	Continuous binary distillation column	[40]
CONTCON	3	Feed rate control of inhibitory substrate in a continuous culture	[21]

(continued)

name	*n*	*background*	*ref*
CR_ELOV	2	Chemical reaction	
CRANE	6	Optimal control of a container crane	[74]
CS_REAC	4	Continuously stirred reactor	[7]
CST_1ORD	2	First order continuous stirred tank with cooling coil	[102]
CSTR	3	Continuous stirred-tank cascade	[40]
CSTR_BM	4	CSTR, benchmark example	[7]
CSTR_CTR	3	Control of continuously stirred tank reactor	[49], [57]
CSTRCOM	5	Isothermal reactor with complex reaction	[40]
DCMDEG	20	Dichloromethane in a biofilm fluidized sand bed	[21]
DEACT	3	Deactivating catalyst in a CSTR	[40]
DEACTENZ	7	Reactor cascade with deactivating enzyme	[21]
DEGEN	2	Notorious academic example, highly degenerate	[10]
DIAUXIA	5	Diauxic growth of a microbe	
DIFDIST	10	Multicomponent differential distillation	[40]
DIODE	2	Tunnel-diode oscillator	[41]
DISLIQU	6	Distribution of substrates in a chemical reactor, liquid phase	
DISPLMNT	3	Displacement curve	
DISRET_O	16	Non-isothermal tubular reactor with axial dispersion	[40]
DISSOC	1	Dissociation kinetics	
DMDS	4	Catalytic conversion of dimethyldisulfide	
DRUGDIS1	2	Time-optimal drug displacement, warfarin and phenylbutazone, one jump	[57], [59]
DRUGDIS2	2	Time-optimal drug displacement, warfarin and phenylbutazone, three jumps	[57], [59]
DRY_FRI1	4	Two-mass oscillator with dry friction between bodies (implicit switching)	[24]
DRY_FRI2	4	Two-mass oscillator with dry friction between bodies, two variable switching times	[24]
DRY_FRI3	4	Two-mass oscillator with dry friction between bodies, four variable switching times	[24]
DUAL	3	Dual substrate limitation	[21]
DUCT	1	Duct design problem (boundary value problem)	[11]
DYNAMO	3	Chaotic behaviour of coupled dynamos	[12], [5]
ENTERO	4	Linear pharmaco-kinetic model with lag-time	
ENZCON	3	Continuous enzymatic reactor	[21]
ENZSPLIT	2	Diffusion and reaction: split boundary solution	[40]
ENZTUBE	1	Tubular enzyme reactor	[21]

(continued)

name	*n*	*background*	*ref*
ENZYM	2	Enzyme effusion problem	[99]
EQBACK	10	Multistage extractor with backmixing	[40]
EQEX	2	Simple equilibrium stage extractor	[40]
EQMULTI	10	Continuous equilibrium multistage extraction	[40]
ETHANOL	4	Ethanol fed-batch fermentation by S. cervisiae	[27]
ETHFERM	7	Ethanol fed batch diauxic fermentation	[21]
EX_BREAK	2	Linear compartment model with application of 2nd dose	
EXO_REAC	4	Exothermic reaction with lag time	
EXOTHERM	2	Exothermic n-th order reaction in closed vessel (normalized)	[100]
EXP_INC	3	Exponentially increasing solutions	[108], [2]
EXP_SIN	1	Exponential-sinus function	[94]
EXP_SOL	2	Exponential solution	[95]
FAST	2	Test problem, fast steady-state	[95], [48]
FBR	8	Fluidized bed recycle reactor	[21]
FED_BAT	2	Optimal feeding strategy for monod-type models by fed-batch experiments	[62]
FED_BATE	2	Optimal feeding strategy for monod-type models by fed-batch experiments, time-dependent feed	[62]
GLOBCO2	7	Global CO2 model, exchange of energy, water, and carbon between continents and atmosphere	[87]
GLUCOSE	3	Glucose reaction	[69]
GLUCOSE1	2	Minimal model for glucose and insulin kinetics	[73]
GLUCOSE2	3	Minimal model for glucose and insulin kinetics	[73]
GOLF	6	Flight of golf ball	[46]
GROWTH_H	1	Logistic growth with stock dependent harvest	[12]
GYROS	7	Idealized gyroscope in terms of quaternions (integral invariant)	[24]
GYROSCOP	3	Heavy symmetric gyroscope	[46]
HIGH_ORD	7	Ordinary differential equation of order 7	
HIRES	8	Growth and differentiation of plant tissue independent of photosynthesis at high levels of irradiance by light	[35]
HOLD	1	Ligament material properties with nonlinear springs and dashpots	
HOLE	1	Academic test example with hole	[94]
HYDROL	2	Batch reactor hydrolysis of acetic anhydride	[40]
IDENT1	2	Structurally globally identifiable model	[103]
IDENT2	1	Gas production by metal dissolution of Volmer-Heyrovski	[103]
IMPULSE	2	Impulse of nerve potential	[90]
INC_STIF	2	Class of test problems with increasing stiffness	[42]

(continued)

name	*n*	*background*	*ref*
INHIB	4	Gas and liquid oxygen dynamics in a continuous fermenter	[21]
INTERLEU	28	Interleukin-13 binding kinetics	[47]
ISO_2PHA	4	Van-de-Vusse reaction in isotherm, ideally mixed CSTR with two phases	
ISO_BAT	4	Ideal isothermal batch reactor	[22]
ISOMER	5	Thermal isomerization of alpha-pinene to dipentene	[98], [13], [88]
ISOTOP1	9	Isotope dilution with nine compartments	
JFIT	1	Chemical reaction	
KATALY1	9	Test reaction for catalysts	
KATALY2	12	Test reaction for catalysts	
KEPLER	4	Modified Kepler problem	[3], [75], [36]
KIDNEY	5	Class of stiff test problems	[86]
KIN_PRO	10	Kinetic chemical process	
KLADYN	4	Dynamic model for KLa	[40]
KNEE	1	Knee problem	[18]
LASER	6	Amplify electro-magnetic radiation by stimulated emission	[6]
LEG_POL	2	Legendre polynomial of order 2	[95]
LEPS	6	LEPS-contour of molecule D-C-H	[85]
LIN_SYS	15	System of linear ODEs	[76]
LINEWEAV	1	Lineweaver-Burk plot	[21]
LKIN	2	Simple linear compartment model	
LKIN_LA	2	Simple linear compartment model with variable lag time	
LKIN_NUM	8	Simple linear compartment model, explicit numerical derivatives	
LKIN_S	8	Simple linear compartment model with sensitivity equations	
LOG_GROW	1	Logistic growth with constant harvest	[12], [55]
LORENZ	3	Lorenz equation	
LORENZ_S	3	Lorenz equation, highly oscillating	[39]
LOT_VOL1	2	Lotka-Volterra differential equation	[39]
LOT_VOL2	2	Lotka-Volterra differential equation	[98]
MARINE	8	Marine population	[19]
MECH_SYS	4	Mechanical oscillating system with elasticity, slack, and damping	
MEMINH	3	Cell retention membrane reactor	[21]
MEMSEP	6	Gas separation by membrane permeation	[40]
MET_SURF	2	Metalloid surface	
METHAN	3	Conversion of methanol to various hydrocarbons	[58]
METHYL	2	Thermal explosion of methyl nitrate (normalized)	[100]
MILK	3	Mastitis with diapedesis of neutrophil	

(continued)

name	n	*background*	*ref*
MINWORLD	3	Mini-world with population, consumption, and environmental pollution	[12], [61]
MIX_RAT1	1	Mixed rate model, chemical reaction	
MIX_RAT3	1	Mixed rate model, chemical reaction (cubic fit for Qd0)	
MIXPOP	3	Predator-prey population dynamics	[21]
MM_META1	4	Metabolic process in urine and plasma, Michaelis-Menten kinetics	[43]
MMKINET	3	Kinetics of enzyme action	[21]
MOISTURE	3	Moisture of granulates	
MOON	1	One-dimensional earth-moon-spaceship problem	[65]
MOTION	4	Motion of a car in a arena	[3]
MUBATCH	8	Multicomponent batch distillation	[40]
MYL_ESTR	4	Methyl ester hydrogenation	[4], [57]
NITRIF	4	Batch nitrification with oxygen transfer	[21]
NITRO	2	Conversion of nitrobenzene to aniline	[40]
NITROGEN	1	Reversible homogeneous gas-phase reaction of nitrogen oxide	[98]
NON_DIFF	2	Simple linear compartment model, non-continuous RHS	
NON_ISO	2	Non-isothermal reactor with time-dependent reactant and temperature	
NON_KIN	2	Nonlinear pharmacokinetic reaction	
NOSTR	3	Non-ideal stirred-tank reactor	[40]
NUTRITI	4	Nutritive cycle with two competing plant populations	[12]
OBSERV1	2	Linear observer in normal form	
OBSERV2	4	Linear observer	
OC_EX3	2	Optimal control test problem	[25], [64]
OC_EX4	2	Optimal control test problem (bang-bang solution)	[25], [64]
OEKOSYS	3	Ecological system with two trophic layers	[52]
OIL	6	Oil shale pyrolysis	[105], [57]
OLIGO	4	Oligosaccharide production in enzymatic lactose hydrolysis	[21]
ON_OFF1	2	On-off kinetics with two lag times	
ON_OFF2	2	On-off kinetics	
ON_OFF3	3	On-off kinetics binding atropin-chase	
ON_OFF4	4	On-off kinetics binding atropin-chase	
ON_OFF5	2	On-off kinetics binding atropin-chase	
ON_OFF6	3	On-off kinetics binding atropin-chase	
ON_OFF7	2	On-off kinetics binding atropin-chase	
OPT_CONT	3	Optimal control problem with 2nd order state constraints	[101], [14]
OPT_KIN	2	Optimal adoption of initial infusion and doses at given therapeutic level	

(continued)

name	*n*	*background*	*ref*
ORB_MOTN	4	Simple orbit motion	[76]
ORBIT	3	Minimum time orbit transfer (optimal control)	[25]
OREGO	3	Belusov-Zhabotinskii reaction (oregonator)	[35], [26]
OSC2INTM	4	Oscillation of the concentration of two intermediates	[32]
OSC_REAC	3	Chemical oscillation	
OSCIL	3	Oscillating tank reactor behavior	[40]
OXDYN	3	Oxygen uptake and aeration dynamics	[21]
OXIDAT	3	Oxidation reaction in an aerated tank	[40]
OZONE	2	Ozon kinetics in atmosphere	[94]
PARTICLE	4	Particle diffusion and reaction (2nd order BVP)	[3]
PEAKS	3	Stiff ODE with sharp peaks	[31]
PEND_ELA	4	Elastic pendulum	[54], [24]
PESTICID	4	Pesticide degradation with explicit microbial population dynamics	[71], [67]
PHA_DYN4	3	Pharmaco-dynamic model with one variable initial lag-time	
PHA_KIN1	3	Linear pharmaco-kinetic model with bolus administration	[37]
PHA_REAC	2	Pharmaco-dynamic reaction	
PHARMA	5	Linear compartmental pharmacological model	
PHB	3	Structured model for PHB production	[21]
PHOSPH_D	3	Chemical reaction, phosphorescence	
PHOTO_PR	1	Daily photoproduction of plants	[12]
PLANT_GR	2	Plant growth (reset of initial values)	
PLASMID	5	Stability of recombinant microorganisms	[21]
POLY1	5	Polymerization	
POLY2	4	Polymerization	
POLYBU	5	Polymerization of high cis polybutadiene in hexane using catalyst	
POLYMER	2	Polymerization	
POPUL	10	Population counts	
PROTOZOA	1	Logistic growth model of protozoa	
PYRIDIN	7	Denitrogenization of pyridin	[9]
RABBIT	2	Rabbits eat grass on an island	
RAMP	1	Ligament material properties with nonlinear springs and dashpots	
RATE_MOD	3	Catalytic hydrodesulfurization of sulfur molecules (DBT)	
RATSOL1	2	Existence of rational solution	[29]
RATSOL2	2	Existence of rational solution	[29]
RE_ENTRY	6	Apollo re-entry problem	[96]
REAC_CTR	2	Control of first-order reversible chemical reaction with dynamic constraints	[45], [56]

(continued)

name	*n*	*background*	*ref*
REACMECH	5	Reaction mechanism with stiff differential equation	[85]
REACTION	5	Chemical reaction	
REFRIG	2	Auto-refrigerated reactor	[40]
REG_RES	2	Dynamics of a population depending on a regenerative resource	[12], [30]
RELAY	2	Simple discontinuous model with a relay	[91]
REVTEMP	4	Reversible reaction with variable heat capacities	[40]
REXT	5	Reaction with integrated extraction of inhibitory product	[40]
ROB_ARM	4	Robot arm with two links	[66]
ROB_CTRL	4	Time-optimal control of two-link robotic arm	[104], [57]
ROBERT	3	Robertson's differential equation for reaction rates	[72]
RODC	2	Radiation from metal rod	[40]
ROESSLER	3	Roessler differential equation	
RUN	4	Relief on a runaway polymerization reaction	[40]
SAT_EXP	3	Saturation experiment in pharmaceutics	
SE	1	Single chemical reaction	
SEMIPAR	5	Parallel reactions in a semi-continuous reactor	[40]
SEMISEQ	5	Sequential reactions in a semi-continuous reactor	[40]
SENS	3	Stiff academic test problem for testing sensitivity analysis	[44]
SHARP1	2	Sharp fronts	[17]
SHARP2	2	Sharp fronts	[17]
SHEEP	9	Transport of radiocaesium in sheep	[28]
SHELL	9	Chemical reaction of aromates	[9]
SIMP_ECO	2	Simple ecological system	[85]
SPBEDRTD	9	Spouted bed reactor mixing model	[40]
SS_TUBE	2	Diffusion-convection in a tube, steady-state	
SSHEATEX	3	Steady-state, two-pass heat exchanger	[40]
STAGED	6	Two-stage culture with product inhibition	[21]
STAR	4	Motion of a star within the potential of a cylindrical galaxy	
STIFF	9	Stiff differential equation	[60]
STIFF_DE	3	Stiff ODE	[93]
STIFF_EQ	2	Stiff ODE	[107]
STIFF1	3	Stiff test problem	[95]
STIFF2	2	Stiff test problem	[95]
SULFUR	5	Radioactive sulfur	
SUPEROX1	1	Dismutation of superoxid ion to H2O and O2	
TAB_DIS1	1	Immediate release of solid dosage forms, extended model	[53]

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