Appendix A

Source Codes

In this appendix, we have collected the source codes of a number of the most important numerical methods for fractional differential equations. This appendix is by no means meant to be comprehensive or complete in any sense: our goal is to provide the reader with a selection of generally applicable easy-to-use programs that should be helpful in a large number of potential applications.

Whereas most of the programs are written in FORTRAN (mainly, standard FORTRAN77), i.e. in a language for which compilers are generally available on almost every conceivable hardware environment, we have also included some Matlab [554], Mathematica [584] and R [555] codes for users who prefer these platforms.

A.1 The Adams-Bashforth-Moulton Method

We begin with the standard version of the Adams-Bashforth-Moulton method with a uniform mesh. The code is divided into a number of subroutines. The first of these computes the required weights.

Algorithm A.1. Computation of the weights of the method. This routine requires an external routine `GAMMA` (such as, e.g., the one provided in [146]) for the evaluation of Euler's Gamma function.

```
      SUBROUTINE ABMW(ALPHA, APRED, ACORR, BCORR, CCORR, N, IERR)
C
C     CALCULATION OF WEIGHTS FOR FRACTIONAL
C     ADAMS-BASHFORTH-MOULTON METHOD
C
```

```
C     INPUT VARIABLES
C     N     - NUMBER OF GRID POINTS
C     ALPHA - ORDER OF DIFFERENTIAL OPERATOR
C
C     OUTPUT VARIABLES
C     APRED  - PREDICTOR WEIGHTS
C     ACORR  - FUNDAMENTAL CORRECTOR WEIGHTS
C     BCORR  - START-POINT CORRECTOR WEIGHTS
C     CCORR  - END-POINT CORRECTOR WEIGHT
C     IERR   - ERROR CODE
C               0 : SUCCESSFUL EXIT
C              12 : ALPHA < 0
C
      IMPLICIT NONE
C
      INTEGER          N, IERR
      DOUBLE PRECISION ALPHA
      DOUBLE PRECISION APRED(N), ACORR(N), BCORR(N), CCORR
C
      INTEGER          J
      DOUBLE PRECISION GMALP1, GMALP2
C
      DOUBLE PRECISION GAMMA
      EXTERNAL         GAMMA
C
      IERR = 0
      IF (ALPHA .LE. 0.D0) IERR = 12
      IF (IERR .NE. 0) RETURN
C
      GMALP1 = GAMMA(ALPHA + 1.D0)
      GMALP2 = GMALP1 * (ALPHA + 1.D0)
C
      CCORR = 1.D0 / GMALP2
C
      DO 100 J = 1, N
         ACORR(J) = ((J+1)**(ALPHA+1.D0) + (J-1)**(ALPHA+1.D0)
     &                - 2 * J**(ALPHA+1.D0)) * CCORR
         APRED(J) = (J**ALPHA - (J-1)**ALPHA) / GMALP1
         BCORR(J) = ((J-1)**(ALPHA+1.D0) - (J-1-ALPHA) * J**ALPHA)
     &               * CCORR
 100  CONTINUE
C
      RETURN
      END
```

The next piece of code demonstrates the application of the Adams-Bashforth-Moulton method, using the weights computed above, by means of a concrete example, namely the initial value problem

$${}^{\mathrm{C}}D^{1.3}y(x) = x^{0.7}E_{1,1.7}(-x) + \exp(-2x) - [y(x)]^2, \quad y(0) = 1,\ y'(0) = -1,$$

where $E_{1,1.7}$ denotes the two-parameter Mittag-Leffler function with parameters 1 and 1.7. The exact solution of this equation is

$$y(x) = \exp(-x).$$

The following program solves this initial value problem with the Adams-Bashforth-Moulton method on the interval $[0, 4]$. The code required here for the evaluation of the Mittag-Leffler function that appears on the right-hand side of the differential equation, *i. e.* the routine `ML2P`, is given in Appendix A.4 below (see Algorithm A.8).

Algorithm A.2. Standard version of the Adams-Bashforth-Moulton method. The algorithm uses the routine `ABMW` from Algorithm A.1 to compute the weights of the method.

```
      SUBROUTINE RHS(X, Y, F)
      IMPLICIT NONE
      DOUBLE PRECISION X, Y, F
C     COMPUTE THE RIGHT-HAND SIDE OF THE DIFFERENTIAL EQUATION
C
      DOUBLE PRECISION ML2P
      EXTERNAL         ML2P
C
      F = X**0.7D0 * ML2P(1.D0, 1.7D0, -X) + EXP(-2.D0*X) - Y**2
      RETURN
      END
C
C
C
      DOUBLE PRECISION FUNCTION EXACT(X)
      IMPLICIT NONE
      DOUBLE PRECISION X
C     COMPUTE THE EXACT SOLUTION
C     OF THE DIFFERENTIAL EQUATION AT THE POINT X
C
      EXACT = EXP(-X)
      RETURN
      END
```

```
C
C
      SUBROUTINE ABMS(ALPHA, N, XMIN, XMAX, RHS, CORRIT, APRED,
     &                BPRED, ACORR, BCORR, CCORR, Y, YO, IERR)
C
C     FRACTIONAL ADAMS METHOD FOR SINGLE CAPUTO FDE OF ORDER ALPHA
C
      IMPLICIT NONE
C
      EXTERNAL         RHS
      INTEGER          N, CORRIT, IERR
      DOUBLE PRECISION ALPHA, XMIN, XMAX, APRED(N), BPRED(N),
     &                 ACORR(N), BCORR(N), CCORR, YO(*), Y(N)
C
C     INPUT VARIABLES (UNCHANGED ON OUTPUT)
C     ALPHA   -  ORDER OF DE, MUST BE > 0.0
C     N       -  NUMBER OF STEPS, MUST BE > 0
C     XMIN    -  LOWER BOUND OF INTERVAL WHERE SOLUTION IS SOUGHT
C     XMAX    -  UPPER BOUND OF INTERVAL WHERE SOLUTION IS SOUGHT,
C                MUST BE > XMIN
C     RHS     -  GIVEN SUBROUTINE THAT COMPUTES THE RHS OF THE DE
C                (SEE BELOW FOR DETAILS)
C     CORRIT  -  NUMBER OF REQUESTED CORRECTOR ITERATIONS
C                (MUST ALWAYS BE >= 1;
C                 IT IS RECOMMENDED TO USE CORRIT = 1
C                 FOR ALPHA >= 1)
C     APRED,BPRED -  PREDICTOR WEIGHTS AS PROVIDED BY WADAMS
C     ACORR,BCORR,CCORR - CORRECTOR WEIGHTS AS PROVIDED BY ABMW
C     YO      -  INITIAL CONDITIONS;
C                YO(J) MEANS (J-1)ST DERIVATIVE OF Y AT XMIN
C
C     OUTPUT VARIABLES
C     Y       -  Y(J) DENOTES APPROXIMATE SOLUTION
C                AT POINT XMIN + J*(XMAX-XMIN)/N
C     IERR    -  ERROR FLAG; WILL BE 0 ON SUCCESSFUL TERMINATION
C
C     THE SUBROUTINE   RHS   MUST HAVE THE FOLLOWING STRUCTURE:
C           SUBROUTINE RHS(X, Y, F)
C           DOUBLE PRECISION X, Y, F
C           INPUT VARIABLES: X, Y
C           OUTPUT VARIABLE: F = F(X,Y)
C     IT MUST BE DECLARED "EXTERNAL" IN THE CALLING SUBROUTINE.
C
C
      DOUBLE PRECISION H, HALP, T, KFAC, WRK(3)
```

```
      INTEGER          J, K, M, CI
C
      IERR = 0
      IF (     N .LE. 0)    IERR = 11
      IF ( ALPHA .LE. 0.D0) IERR = 12
      IF (CORRIT .LE. 0)    IERR = 14
      IF (  XMAX .LE. XMIN) IERR = 15
      IF (IERR .NE. 0) RETURN
C
      H    = (XMAX - XMIN) / N
      HALP = H ** ALPHA
      M    = INT(ALPHA)
      IF (ALPHA .EQ. DBLE(M)) M = M - 1
C
      DO 1000 J = 1, N
         T = XMIN + J * H
C
C        SET INITIAL CONDITION
         WRK(1) = Y0(1)
         KFAC = 1.D0
         DO 50 K = 1, M
            KFAC = KFAC * K
            WRK(1) = WRK(1) + T**K / KFAC * Y0(K+1)
 50      CONTINUE
C
C        PREDICTOR
         CALL RHS(XMIN, Y0(1), WRK(3))
         WRK(2) = WRK(1) + HALP * BPRED(J) * WRK(3)
         DO 70 K = 1, J-1
            CALL RHS(XMIN + (J-K)*H, Y(J-K), WRK(3))
            WRK(2) = WRK(2) + HALP * APRED(K) * WRK(3)
 70      CONTINUE
C
C        CORRECTORS
         CALL RHS(XMIN, Y0(1), WRK(3))
         WRK(1) = WRK(1) + HALP * BCORR(J) * WRK(3)
         DO 110 K = 1, J-1
            CALL RHS(XMIN + (J-K)*H, Y(J-K), WRK(3))
            WRK(1) = WRK(1) + HALP * ACORR(K) * WRK(3)
 110     CONTINUE
         DO 120 CI = 1, CORRIT
            CALL RHS(T, WRK(2), WRK(3))
            WRK(2) = WRK(1) + HALP * CCORR * WRK(3)
 120     CONTINUE
C
         Y(J) = WRK(2)
```

```
C
 1000 CONTINUE
C
      RETURN
      END
C
C
C
      PROGRAM EXAMPL
      IMPLICIT NONE
C
      DOUBLE PRECISION Y0(2), Y(40), XMIN, XMAX, ALPHA, X,
     &                 APRED(40), ACORR(40), BCORR(40), CCORR,
     &                 EXACT
      INTEGER          J, K, N, CORRIT, IERR
      EXTERNAL         RHS, EXACT
C
C     DEFINE PARAMETERS OF EQUATION
      ALPHA = 1.3D0
      XMIN = 0.D0
      XMAX = 4.D0
C
C     DEFINE INITIAL CONDITIONS
      Y0(1) =  1.D0
      Y0(2) = -1.D0
C
C     DEFINE PARAMETERS OF NUMERICAL METHOD
C     MAXIMUM NUMBER OF GRID POINTS
      N = 40
C     NUMBER OF CORRECTOR ITERATIONS ACCORDING TO RECOMMENDATION
      CORRIT = 1
C
C     COMPUTE WEIGHTS
      CALL ABMW(ALPHA, APRED, ACORR, BCORR, CCORR, N, IERR)
      IF (IERR .NE. 0) THEN
         WRITE(*,'(A,I4)') 'ERROR IN COMPUTATION OF WEIGHTS: ', IERR
         STOP
      END IF
C
C     SOLVE EQUATION NUMERICALLY WITH 10, 20, 40 GRID POINTS
      DO 100 J = 1, 3
         N = 5 * 2**J
         CALL ABMS(ALPHA, N, XMIN, XMAX, RHS, CORRIT,
     &              APRED, APRED, ACORR, BCORR, CCORR, Y, Y0, IERR)
         IF (IERR .NE. 0) THEN
            WRITE(*, '(A,I3,A,I3)') 'ERROR CODE ', IERR,
```

```
     &               ' IN DIFFERENTIAL EQUATION SOLVER FOR N =', N
          ELSE
             WRITE(*, '(A)') '=========================='
             WRITE(*, '(A,I3)') 'NUMBER OF GRID POINTS: ', N
             WRITE(*, '(A)')
     &           'X       EXACT VALUE   APPROX. VALUE       ERROR'
             DO 50 K = 1, N
                X = XMIN + (XMAX-XMIN) / DBLE(N) * DBLE(K)
                WRITE (*, '(F6.4,F13.6,F16.6,F12.6)')
     &              X, EXACT(X), Y(K), EXACT(X) - Y(K)
 50          CONTINUE
          END IF
 100   CONTINUE
       END
```

Next we provide the parallel version of the method as developed in [173]. It uses the OpenMP programming model [434] for the parallelization. The particular example implemented here solves the initial value problem

$$ {}^{\mathrm{C}}D^{\alpha}y(x) = -y(x), \qquad y(0) = 1, \quad y'(0) = 0, $$

on an interval $[0, X]$. The program should be called with three parameters, namely α (the order of the differential operator which must be in the interval $(0, 2]$; the second of the two initial conditions above is only used if $\alpha > 1$), the number of grid points, and X, the right end point of the interval of interest.

Algorithm A.3. OpenMP-based parallel version of the Adams-Bashforth-Moulton method. The algorithm uses the routine `ABMW` from Algorithm A.1 to compute the weights of the method.

```
      SUBROUTINE ABMSP(ALPHA, N, XMIN, XMAX, RHS, CORRIT,
     &                 APRED, BPRED, ACORR, BCORR, CCORR, Y, Y0,
     &                 WRK, IERR)
C
C     FRACTIONAL ADAMS METHOD FOR SINGLE CAPUTO FDE OF ORDER ALPHA
C     PARALLELIZED WITH OPENMP
C
      IMPLICIT NONE
C
      EXTERNAL         RHS
      INTEGER          N, CORRIT, IERR, FNSHD
      DOUBLE PRECISION ALPHA, XMIN, XMAX, APRED(N), BPRED(N),
```

```
     &                 ACORR(N), BCORR(N), CCORR, YO(*), Y(N),
     &                 WRK(N)
C
C     INPUT VARIABLES (UNCHANGED ON OUTPUT)
C     ALPHA   -  ORDER OF DE, MUST BE > 0.0
C     N       -  NUMBER OF STEPS, MUST BE > 0
C     XMIN    -  LOWER BOUND OF INTERVAL WHERE SOLUTION IS SOUGHT
C     XMAX    -  UPPER BOUND OF INTERVAL WHERE SOLUTION IS SOUGHT,
C                MUST BE > XMIN
C     RHS     -  GIVEN SUBROUTINE THAT COMPUTES THE RHS OF THE DE
C                (SEE BELOW FOR DETAILS)
C     CORRIT  -  NUMBER OF REQUESTED CORRECTOR ITERATIONS
C                (MUST ALWAYS BE >= 1;
C                 RECOMMENDATION: USE CORRIT = 1 FOR ALPHA >= 1)
C     APRED,BPRED -  PREDICTOR WEIGHTS AS PROVIDED BY ABMW
C     ACORR,BCORR,CCORR - CORRECTOR WEIGHTS AS PROVIDED BY ABMW
C     YO      -  INITIAL CONDITIONS;
C                YO(J) MEANS (J-1)ST DERIVATIVE OF Y AT XMIN
C
C     OUTPUT VARIABLES
C     Y       -  Y(J) DENOTES APPROXIMATE SOLUTION
C                AT POINT XMIN + J*(XMAX-XMIN)/N
C     WRK     -  WORKSPACE
C     IERR    -  ERROR FLAG; WILL BE 0 ON SUCCESSFUL TERMINATION
C
C     THE SUBROUTINE   RHS   MUST HAVE THE FOLLOWING STRUCTURE:
C           SUBROUTINE RHS(X, Y, F)
C           DOUBLE PRECISION X, Y, F
C           INPUT VARIABLES: X, Y
C           OUTPUT VARIABLE: F = F(X,Y)
C     IT MUST BE DECLARED "EXTERNAL" IN THE CALLING SUBROUTINE.
C
      DOUBLE PRECISION H, HALP, T, KFAC, ICND, PRD, CRR, F, WO
      INTEGER          B, J, K, M, CI, I
      INTEGER          NBLKS, OMPNTH,
     &                 OMP_GET_NUM_THREADS, OMP_GET_THREAD_NUM
      EXTERNAL         OMP_GET_NUM_THREADS, OMP_GET_THREAD_NUM
C
      IERR = 0
      IF (     N .LE. 0)    IERR = 11
      IF ( ALPHA .LE. 0.D0) IERR = 12
      IF (CORRIT .LE. 0)    IERR = 14
      IF (  XMAX .LE. XMIN) IERR = 15
      IF (IERR .NE. 0) RETURN
C
      H    = (XMAX - XMIN) / N
```

```
      HALP = H ** ALPHA
      M    = INT(ALPHA)
      IF (ALPHA .EQ. DBLE(M)) M = M - 1
C
      CALL RHS(XMIN, Y0(1), W0)
      W0 = W0 * HALP
      FNSHD = 0
C
C
!$OMP    PARALLEL PRIVATE(I, J, K, ICND, KFAC, NBLKS,
!$OMP&                     T, PRD, CRR, CI, F, B)
!$OMP&            SHARED (OMPNTH, N, H, XMIN, Y0, M, APRED,
!$OMP&                    ACORR, BCORR, CCORR, WRK, Y, CORRIT,
!$OMP&                    HALP, FNSHD, W0)
C
      OMPNTH = OMP_GET_NUM_THREADS()
      NBLKS = CEILING(DBLE(N)/DBLE(OMPNTH))
C
      DO 1000 B = 0, NBLKS - 1
C
!$OMP    DO
C
         DO 2000 I = 1, OMPNTH
            J = B * OMPNTH + I
            IF (J .LE. N) THEN
               T = XMIN + J * H
C
C              SET INITIAL CONDITION
               ICND = Y0(1)
               KFAC = 1.D0
               DO 50 K = 1, M
                  KFAC = KFAC * K
                  ICND = ICND + T**K / KFAC * Y0(K+1)
 50            CONTINUE
C
C              PREDICTOR AND CORRECTOR: FIRST PART OF SUMMATION
               PRD = ICND + BPRED(J) * W0
               CRR = ICND + BCORR(J) * W0
               DO 70 K = J - B * OMPNTH, J - 1
                  PRD = PRD + APRED(K) * WRK(J-K)
                  CRR = CRR + ACORR(K) * WRK(J-K)
 70            CONTINUE
C
               DO 80 K = I-1, 1, -1
                  DO WHILE (FNSHD .LT. J-K)
!$OMP                FLUSH (Y, WRK, FNSHD)
```

```
                  END DO
                  PRD = PRD + APRED(K) * WRK(J-K)
                  CRR = CRR + ACORR(K) * WRK(J-K)
 80            CONTINUE
C
C              CORRECTORS: PROPER CORRECTOR ITERATIONS
               DO 120 CI = 1, CORRIT
                  CALL RHS(T, PRD, F)
                  PRD = CRR + HALP * CCORR * F
 120           CONTINUE
C
               Y(J) = PRD
               CALL RHS(T, Y(J), WRK(J))
               WRK(J) = WRK(J) * HALP
               FNSHD = J
!$OMP          FLUSH (Y, WRK, FNSHD)
C
         ENDIF
C
 2000    CONTINUE
!$OMP    END DO
C
 1000 CONTINUE
!$OMP END PARALLEL
      RETURN
      END
C
C
      SUBROUTINE RHS (X, Y, F)
      IMPLICIT NONE
      DOUBLE PRECISION X, Y, F
      F = -1.D0 * Y
      RETURN
      END
C
C
C     EXAMPLE MAIN PROGRAM
C
      PROGRAM PARFDE
C
      IMPLICIT NONE
C
      INTEGER MAXPTS
      PARAMETER (MAXPTS=1000000)
C
      INTEGER IARGC
```

```
C
      DOUBLE PRECISION YO(2), Y(MAXPTS), XMIN, XMAX, ALPHA, X,
     &                 APRED(MAXPTS), ACORR(MAXPTS), BCORR(MAXPTS),
     &                 CCORR, WRK(MAXPTS)
      INTEGER          K, N, CORRIT, IERR, NPTS
      EXTERNAL         RHS, IARGC, GETARG
      CHARACTER *72    ARGV
C
      N = IARGC()
      IF (N .NE. 3) THEN
         WRITE (*, '(A)') 'WRONG NUMBER OF ARGUMENTS.'
         WRITE (*, '(A)') 'USAGE: PARFDE ALPHA NPTS XMAX'
         STOP
      ENDIF
C
      CALL GETARG (1, ARGV)
      READ (ARGV, *) ALPHA
      CALL GETARG (2, ARGV)
      READ (ARGV, *) NPTS
      IF (NPTS .GT. MAXPTS) THEN
         WRITE (*, '(A,I,A,I,A)') 'TOO MANY POINTS: ', NPTS,
     &                    '(MAX: ', MAXPTS, ')'
         STOP
      ENDIF
      CALL GETARG (3, ARGV)
      READ (ARGV, *) XMAX
C
C     DEFINE PARAMETERS OF EQUATION
      XMIN = 0.D0
C
C     DEFINE INITIAL CONDITIONS
      YO(1) = 1.D0
      YO(2) = 0.D0
C
C     DEFINE PARAMETERS OF NUMERICAL METHOD
      CORRIT = 1
C
C     COMPUTE WEIGHTS
      CALL ABMW(ALPHA, APRED, ACORR, BCORR, CCORR, NPTS, IERR)
      IF (IERR .NE. 0) THEN
         WRITE (*, '(A,I4)') 'ERROR IN COMPUTATION OF WEIGHTS: ',
     &                       IERR
         STOP
      END IF
C
C     SOLVE EQUATION NUMERICALLY
```

```
      CALL ABMSP(ALPHA, NPTS, XMIN, XMAX, RHS, CORRIT, APRED,
     &           APRED, ACORR, BCORR, CCORR, Y, Y0, WRK, IERR)
      IF (IERR .NE. 0) THEN
         WRITE (*, '(A,I3,A,I3)') 'ERROR CODE ', IERR,
     &             ' IN DIFFERENTIAL EQUATION SOLVER FOR NPTS = ',
     &             NPTS
      ELSE
         WRITE(*, '(A,F14.6)') 'ALPHA = ', ALPHA
         WRITE(*, '(A,I14)')   'NPTS  = ', NPTS
         WRITE(*, '(A,F14.6)') 'XMAX  = ', XMAX
         WRITE(*, '(A)') '=========================='
         WRITE(*, '(A)')
     &        '          X          APPROX. VALUE'
         DO 50 K = 1, NPTS
            X = XMIN + (XMAX-XMIN) / DBLE(NPTS) * DBLE(K)
            WRITE (*, '(F16.8,F19.12)') X, Y(K)
 50      CONTINUE
      END IF
 100  CONTINUE
C
      END
```

A.2 Lubich's Fractional Backward Differentiation Formulas

For the fractional backward differentiation formulas introduced by Lubich, we here list the Matlab implementations due to Weilbeer [576]. This implementation consists of three separate routines. The first of these routines computes the solution at the starting points of the grid.

Algorithm A.4. Matlab implementation of Lubich's fractional BDF: Starting points.

```
function[Y] = startpoints(C,S,a,y0,alpha,T)
% STARTPOINTS solves the nonlinear equation system for the first
%   a values of the fractional differential equation
%
%   (1)    D^{\alpha} * y(t) = f(t,y(t))
%
%   using a simple Newton method with a start solution corresponding
%   to the initial condition of (1).
%
%   Input Data:
%   -----------
```

```
%   C    - Convolution weights vector
%   S    - Starting weights matrix
%   a    - number of start weights
%   alpha  - Order of FDE alpha \in (0,1)
%   T    - mesh
%   y0    - Initial conditions
%
%   Output Data:
%   ------------
%   Y    - Solution at a-1 points
%
%   Note:
%   -----
%   This is not a stand-alone function but a subroutine of FBDFP.m

h = T(2)-T(1);
Y = y0(1).*ones(a-1,1);
IC= fliplr(y0); % Initial conditions polynomial

syms y t;

% right-hand side diff w.r.t. y
fj = inline(char(diff(rhs(t,y,alpha),y)),'t','y');
% right-hand side
ff = inline(char(rhs(t,y,alpha)),'t','y');

B = 1/h^alpha*(rot90(hankel(fliplr(C(1:a)))) + S(1:a,1:a));

% Evaluation of the initial conditions polynomial
P = polyval(IC,T(2:a));

B = B(2:a,2:a);
Pp = B*P';

er = 1;

while er > 1e-8
   for k=1:a-1
      Fj(k) = fj(T(k+1),Y(k));
      Ff(k) = ff(T(k+1),Y(k))+Pp(k);
   end
   X = (B - diag(Fj))\(B*Y - Ff');
   er = abs(max(X));
   Y = Y-X;
end
```

The second routine is devoted to the construction of the matrix that contains the weights of the method. Recall that a linear system of equations needs to be solved in this context; the parameter c of the subroutine allows the user to choose between various alternative numerical methods for the solution of this linear system.

Algorithm A.5. Matlab implementation of Lubich's fractional BDF: Computation of weights.


```
function[C, S, a, r] = ltsmp(N,alpha,p,c)
% LTSMP(N,alpha,p,c)
%   LTSMP creates the p-th order lower triangular strip matrix
%   corresponding to the discrete approximation of the fractional
%   differential or integral operator D^alpha at N nodes.
%
%   Input Data:
%   -----------
%   N      - number of nodes of the discretization.
%   alpha  - order of the fractional integration / differentiation.
%            alpha > 0 means integration,
%            alpha < 0 means differentiation.
%            abs(alpha) < 1.
%   p      - order of approximation
%            (between 1 and 6 for stability reasons).
%   c      - choice of numerical method for the
%            calculation of the starting weights.
%       'lu'      - solution of the equation system
%                         using lu decomposition
%       'lui'     - computation of the inverse using
%                         lu decomposition of wcoeff followed by
%                         matrix multiplication A^(-1)*rhs
%       'gmres'   - gmres solution of the equation system
%       'gmresi'  - inverse using gmres ...
%       'gmresh'  - gmres solution of the equation system using
%                         Householder orthogonalization
%       'qr'      - solution of the equation system using
%                         QR decomposition
%       'svd'     - solution of the equation system using SVD
%       'bpi'     - inverse using Bjoerck-Pereyra Algorithm
%                         (alpha has to be a unit fraction
%                         for this choice)
%
%   Output Data:
%   ------------
%   <C>    - Vector with N convolution weights
```

```
%             (omega_0,omega_1,...,omega_N-1)
%   <S1>    - Matrix with N*a starting weights:
%             [ w_0,1  w_0,2  w_0,3 ... w_0,a ]
%             [ w_1,1  w_1,1  w_1,2 ... w_1,a ]
%             [       . . .       ]
%             [ w_N-1,1      . . .    w_N-1,a ]
%   <a>     - Number of starting weights for each n.
%   <r>     - average residual of the start weight computation
%             over all right hand sides.

% Error handling.

if nargin ~= 4
   error('Wrong number of input arguments.')
end

% Calculating length(a) and q (=gamma).
cnt = 1;
q   = 0;
for k=0:p-1
   for l=0:ceil(1/abs(alpha)).*(p-1)
      qt = k+l*abs(alpha);  % potential gamma value.
      de = find(chop(q,10)==chop(qt,10)); % Avoid double entries.
      if qt <= p-1 & isempty(de) == 1
 cnt = cnt+1;
 q(cnt) = qt;
      end
   end
end
% Sort feasible gamma entries in increasing order.
q = sort(q);
[nil, a] = size(q);        % Counting number of starting weights.

% Convolution weights (via automatic differentiation).
U = zeros(6,N);
U(1:6,1:7) =   [ 1      -1    0      0     0     0    0;
                 3/2    -2   1/2     0     0     0    0;
                11/6    -3   3/2   -1/3    0     0    0;
                25/12   -4    3    -4/3   1/4    0    0;
               137/60   -5    5   -10/3   5/4  -1/5   0;
               147/60   -6  15/2  -20/3  15/4  -6/5  1/6 ];

C(1) = U(p,1)^(-alpha);
for s=1:N-1
   tmp = zeros(1,p+1);
   if s < p+2
```

```
      for v=0:s-1
         tmp(v+1) = (alpha*(v-s)-v)*C(v+1)*U(p,s-v+1);
      end
      C(s+1) = 1/(s*U(p,1)) * sum(tmp);
   else
      for v=s-(p+1):s-1
         tmp(v-(s-(p+1))+1) = (alpha*(v-s)-v)*C(v+1)*U(p,s-v+1);
      end
      C(s+1) = 1/(s*U(p,1)) * sum(tmp);
   end
end

% Starting weights
if p ~= 1   % if p=1 no additional starting weights are needed

   % Exact fractional integrals
   s(1,1:a) = gamma(1+q(1,1:a))./gamma(1+q(1,1:a)+alpha);

   % Right-hand sides
   for k=1:a
      T(1:N) = (1:N).^q(1,k);
      L(1:N-1) = (1:N-1).^(q(1,k)+alpha);
      Y = conv(C,T);
      rhs(2:N,k) = s(1,k)'*L(1:N-1)' - Y(1:N-1)';
   end

   % Coefficient Matrix
   for k=1:a
      Wcoeff(k,:) = (0:a-1).^q(1,k);
   end

   switch lower(c)

      case 'lu'
      % 1) Solution of the linear equation systems
      %    using the \ operator
      S(1:N,:) = (Wcoeff\rhs(1:N,:)')';

      case 'lui'
      % 2) Solution of the linear equation systems
      %    using the inverse
      Wcoeffinv = inv(Wcoeff);
      S(1:N,:) = (Wcoeffinv*rhs(1:N,:)')';

      case 'gmres'
      % 3) Solution using gmres at each step
```

```
%    on the actual system.
for k=1:N
   [S(:,k), flag,relres,iter]
       = gmres(Wcoeff,rhs(k,:)',a+1,1e-16,1);
end
S = S';

case 'gmresi'
% 4) Computing the inverse of Wcoeff using gmres
for k=1:a
   unitVector = zeros(a,1);
   unitVector(k,1) = 1;
   [Wcoeffinv(:,k), flag]
      = gmres(Wcoeff,unitVector,a+1,1e-16,1);
end
for k=1:N
   S(k,:) = (Wcoeffinv*rhs(k,:)')';
end

case 'gmresh'
% 5) Solution using gmreshouseholder at each step
%    on the actual system.
for k=1:N
   S(:,k)
      = gmresh(Wcoeff,rhs(k,:)',zeros(a,1),1e-32,a);
end
S = S';

case 'qr'
% 6) Solution using QR decomposition.
[Q R] = qr(Wcoeff);
S(1:N,:) = (R\(Q'*rhs(1:N,:)'))';

case 'svd'
% 7) Solution using SVD.
S = zeros(N,a);
[Uv Sv Vv] = svd(Wcoeff);
for l=1:N
   for k=1:a
      S(l,:) = S(l,:)
                + (Uv(:,k)'*rhs(l,:)'*Vv(:,k)./Sv(k,k))';
   end
end

case 'bpi'
% 8) Calculating the inverse using the Bjoerck-Pereyra
```

```
      %    algorithm (alpha has to be a unit fraction)
      [num, num2] = rat(alpha);
      if abs(num) ~= 1
         fprintf(1,
             '\n alpha is not a unit fraction. Cannot use bpi\n');
      else
         X = (0:a-1).^(abs(alpha));
         % Calculating the inverse
         Wcoeffinv = bpif(X,'p');
         % Solving for the N right-hand sides
         S(1:N,:) = (Wcoeffinv*rhs(1:N,:)')';
      end

      otherwise
      fprintf(1,
         '\n Wrong choice for parameter c.\n');
   end
   % residual tester
   Residual(1:N,1) = norm(Wcoeff*S(1:N,:)'- rhs(1:N,:)');
   r = sum(abs(Residual))/length(Residual);

else
   a = 1;
   S = zeros(N,1);
   r = 0;
end

fprintf(1,'\n The average residual is %g.\n',r);
```

Finally we give the main part of the algorithm that actually computes the required approximate solutions, using the two auxiliary routines listed above.

Algorithm A.6. Matlab implementation of Lubich's fractional BDF: Main part.

```
function[Y] = fbdfp(N,alpha,y0,b,p,in,ie,c)

% FBDFP(N,alpha,y0,b,p,in,ie,c)
%   Fractional Backward Difference Formula of order p.
%   FBDFP solves the fractional order differential equation (FDE)
%
%   (1)    D^alpha * y(t) = f(t,y(t))  ,alpha \in (0,1)
%
%   at N equispaced mesh points on the interval [0,b].
```

```
%   The method has a theoretical convergence order of p. The
%   parameters 'in' (iteration number) and 'ie' (iteration error)
%   determine the maximal number of iterations or the minimal
%   change of two consecutive iterations at each mesh points.
%   The parameter c determines the numerical method used to generate
%   the discretized fractional differential operator D^alpha.
%   The right-hand side of (1) has to be stored in an external
%   matlab function in the file rhs.m.
%
%   Input Data:
%   -----------
%   N      - Number of mesh points.
%   alpha  - Order of FDE alpha \in (0,1).
%   b      - Right interval end (0 assumed to be left start).
%   y0     - Starting values y^(k)(0) = c_k as vector
$            y0 = [c_0, c_1, ... , c_k].
%   p      - desired convergence order (p = 1-6).
%   in     - Maximal number of iteration at each mesh point.
%   ie     - Minimal change of two consecutive iteration steps.
%   c      - choice of numerical method for the calculation
%            of the starting weights
%
%   rhs.m  - externally stored right-hand side f(t,y(t)) of FDE.
%
%   Output Data:
%   ------------
%   Y      - Solution at the N mesh points.
%
%   See also FBDFPS, LTSMP, LTSMPS, RHS, STARTPOINTS.

if nargin ~= 8
   error('Wrong number of input arguments.')
end

Y      = zeros(N,1);                  % Solution.
Yt     = zeros(N,1);                  % Auxiliary variables.
Z      = zeros(N,1);

Y(1,1) = y0(1);                       % Initial Conditions.
IC     = fliplr(y0);

T = linspace(0,b,N);                  % Equidistant mesh points.
h = T(2)-T(1);                        % Step size.
[C S a] = ltsmp(N,-alpha,p,c);        % Calculating lower
                                      % triangular strip matrix.
```

```
if p ~= 1
   Sp = startpoints(C,S,a,y0,alpha,T); % Startpoints calculation.
   Y(2:a) = Sp(1:a-1);                 % Setting start values.
end

for k=1+a:N

   K  = zeros(1,k);
   Ym = Y(1:k);
   ICm(1:k) = polyval(IC,T(1:k));

   K(1:k) = C(k:-1:1);
   K(1:a) = K(1:a) + S(k,1:a);

   St = 1/C(1).*K*Ym;
   A  = 1/C(1).*K*ICm';

   % First guess using previous solution point

   Z(k) = (h^(alpha))/C(1)*rhs(T(k),Y(k-1),alpha) - St + A;

   er = 5;                       % auxiliary variables for iteration.
   cnt = 1;

   while er >= ie & cnt < in     % Fixed point iteration.
      Yt(k) = (h^(alpha))/C(1)*rhs(T(k),Z(k),alpha) - St + A;
      er    = abs(Yt(k)-Z(k));
      Z(k)  = Yt(k);
      cnt   = cnt+1;
   end

   Y(k) = Z(k);

   if imag(Y(k)) ~= 0            % termination criterion.
      Y(k:N) = 0;
      break;
   end

end
```

A.3 Time-fractional Diffusion Equations

Our last differential equation solver is a finite difference method for a time-fractional diffusion equation

$$ {}^{\mathrm{C}}D_t^{\alpha} y(x,t) + \Phi(x,t)\frac{\partial^2}{\partial x^2} y(x,t) = f(x,t), \qquad x \in [a,b], \quad t \in [0,T], $$

with $0 < \alpha < 1$, the initial condition

$$ y(x,0) = y_0(x) $$

and mixed Dirichlet-Neumann boundary conditions

$$ g_1(t)y(a,t) + h_1(t)\frac{\partial}{\partial x} y(a,t) = r_1(t), $$
$$ g_2(t)y(b,t) + h_2(t)\frac{\partial}{\partial x} y(b,t) = r_2(t) $$

as discussed in Subsection 3.2.2. This algorithm is given in a form suitable for direct use within the Mathematica software package [584]. It is based on the approximation developed in Eqs. (2.1.10) and (2.1.11) for the fractional derivative with respect to t, using a stepsize of $\Delta t = T/n_t$, and on a standard centered difference approximation with step size $\Delta x = (b-a)/n_x$ for the second-order derivative with respect to x, where n_t and n_x are preassigned positive integers.

The algorithm requires that $\Phi(a,t) \neq 0$ and $\Phi(b,t) \neq 0$ for all $t \in [0,T]$. The algorithm computes (n_x+1)-dimensional vectors `u[0]`, `u[1]`, ..., `u[`n_t`]` (in Mathematica notation) with the interpretation that the component `u[k][[j]]` is the approximation of the exact solution $y((j-1)\cdot\Delta_x, k\cdot\Delta_t)$ where $k \in \{0,1,\ldots n_t\}$ and $j \in \{1,2,\ldots,n_x+1\}$.

Algorithm A.7. Mathematica implementation of a backward differentiation method for the solution of the time-fractional diffusion equation in one space dimension.

```
(* Load package for handling of tridiagonal linear systems *)
<< LinearAlgebra`Tridiagonal`

(* Initialize parameters of the equation (given data) *)
```

```
(* boundaries of intervals *)
(* values are to be understood as examples *)
a = 0;
b = 1;
T = 1;

(* functions in boundary conditions *)
(* values are to be understood as examples *)
r1[t_] := 0;
r2[t_] := 1;
g1[t_] := 1;
g2[t_] := 1;
h1[t_] := 0;
h2[t_] := 0;

(* function in initial condition *)
(* value is to be understood as example *)
u0[x_] := x;

(* functions in the differential equation itself *)
(* values are to be understood as examples *)

phi[x_, t_] := -1;
f[x_, t_] := 0;

(* order of fractional differential operator with respect to time *)

alpha = 0.5;
Clear[weight];

(* initialize parameters of the numerical scheme:
   number of steps in coordinate directions *)
(* values for nx and nt are to be understood as examples *)
nx = 67;
nt = 80;
deltax = (b - a)/nx;
deltat = T/nt;

(* auxiliaries *)
ga = Gamma[2 - alpha];

(* define weights of fractional BDF *)
weight[j_, k_] := weight[j, k] = Which[j == 0, 1,
    j == k, k^(-alpha) (1 - alpha - k) + (k - 1)^(1 - alpha),
    True, (j - 1)^(1 - alpha) -
     2 j^(1 - alpha) + (j + 1)^(1 - alpha)]/ga
```

```
(* main part of algorithm *)

(* assign initial values *)

u[0] = Table[u0[a + (j - 1) deltax], {j, 1, nx + 1}];

(* time step loop *)
Do[
 tk = k deltat;

 (* construction of tridiagonal matrix of linear system
    for each time step *)
 lower =
  Append[Table[phi[a + j deltax, tk], {j, 1, nx - 1}],
           -h2[tk]] / deltax^2;
 main = Append[
   Prepend[Table[-2 phi[a + j deltax, tk] / deltax^2 +
      weight[0, k] / deltat^alpha, {j, 1, nx - 1}],
    g1[tk] / deltax +
     h1[tk] (-1/deltax^2 + 1/(2 ga deltat^alpha phi[a, tk] ))],
   g2[tk] / deltax +
    h2[tk] (1/deltax^2 - 1/(2 ga deltat^alpha phi[b, tk] ))];
 upper = Prepend[Table[phi[a + j deltax, tk], {j, 1, nx - 1}],
    h1[tk]]/deltax^2;

 (* construction of vector on right-hand side of system *)
 rhs = Prepend[
   Append[
    Table[f[a + j deltax, tk]
           + u[0][[j]] (1 - alpha) /ga/tk^alpha
           - Sum[weight[mu, k] u[k - mu][[j]], {mu, 1, k}] /
                 deltat^alpha, {j, 2, nx}],
    r2[tk]/deltax -
     0.5 h2[tk] / phi[b, tk] (
       f[b, tk] + u0[b] tk^(-alpha) (1 - alpha)/ga
        - Sum[weight[mu, k] u[k - mu][[nx + 1]], {mu, 1, k}]/
         deltat^alpha)],
    r1[tk]/deltax +
    0.5 h1[tk] / phi[a, tk] (
      f[a, tk] + u0[a] tk ^(-alpha) (1 - alpha)/ga
       - Sum[weight[mu, k] u[k - mu][[1]], {mu, 1, k}]
           / deltat^alpha)];

 (* approximate solution at present time step is obtained
    by solving this tridiagonal system *)
```

```
 u[k] = TridiagonalSolve[lower, main, upper, rhs]
, {k, 1, nt}]
```

A.4 Computation of the Mittag-Leffler Function

In this section, we give a fast routine for the computation of the two-parameter Mittag-Leffler function $E_{\alpha,\beta}(x)$ for $\alpha \geq 0$, $\beta > 0$ and real values of x. The routine has been developed to run fast; its accuracy is very high only for $x \leq 1$. If highly accurate results are required for $x > 1$ or for complex arguments x then we recommend to use the routine of Gorenflo *et al.* [247, 248]. A Matlab version of such a code is available [455].

Algorithm A.8. FORTRAN77 implementation of a routine for the fast evaluation of two-parameter Mittag-Leffler functions. This routine requires an external routine `GAMMA` (such as, e.g., the one provided in [146]) for the evaluation of Euler's Gamma function.

```
      DOUBLE PRECISION FUNCTION ML2P(ALPHA, BETA, X)
C
      IMPLICIT NONE
      DOUBLE PRECISION ALPHA, BETA, X
C
C     FAST COMPUTATION OF TWO-PARAMETER MITTAG-LEFFLER FUNCTION
C
C     PARAMETERS
C     ALPHA - INPUT - FIRST PARAMETER OF MITTAG-LEFFLER FUNCTION
C     BETA  - INPUT - SECOND PARAMETER OF MITTAG-LEFFLER FUNCTION
C     X     - INPUT - ARGUMENT OF THE MITTAG-LEFFLER FUNCTION
C
      INTEGER          K, IERR
      DOUBLE PRECISION TMP, NEW, GMARG, GAMMA
      EXTERNAL         GAMMA
C
      TMP = 1.D0 / GAMMA(BETA)
      K = 1
C
 100  GMARG = ALPHA * K + BETA
      NEW =  X**K / GAMMA(GMARG)
      TMP = TMP + NEW
      K = K + 1
      IF (GMARG .LT. 5.D0) GOTO 100
      IF (K .LT. 100  .AND.  ABS(NEW) * 1.D16 .GT. TMP) GOTO 100
```

```
C
      ML2P = TMP
C
      RETURN
      END
```

A.5 Monte Carlo Simulation of CTRW

We conclude this appendix with two implementations (in R and in Matlab) of a Monte Carlo program to simulate CTRWs according to the algorithm described in section 7.3. The program below generates and plots a single realization of a CTRW with a given number of jumps and durations. Even if this is a very simple algorithm, it consists of three parts. The first part is the generator of independent and indentically distributed Mittag-Leffler deviates according to equation 7.3.2. Then, Lévy α-stable deviates are generated following equation 7.3.1. Finally, cumulative sums give the position coordinates and the epochs and positions are plotted as a function of the epochs. This routine can be easily modified with suitable external cycles to generate many realizations up to a given time t and estimate the probability density $f_{X(t)}(x,t)$ from the histogram of realized positions $X(t)$. This was explicitly done in reference [231].

Algorithm A.9. Matlab implementation for the Monte Carlo simulation of CTRW.

```
%Plot of a single CTRW realization

%Generation of Mittag-Leffler deviates
%See Fulger, Scalas, Germano 2008 and references therein

n=100; %number of points
gammat=1; %scale parameter
beta=0.99; %ML parameter

u1=rand(n,1); %uniform deviates
v1=rand(n,1); %uniform deviates

%Generation of symmetric alpha stable deviates

tau=-gammat*log(u1).*(sin(beta*pi).
/tan(beta*pi*v1)-cos(beta*pi)).^(1/beta);
```

```
gammax=1; %scale parameter
alpha=1.95; %Levy parameter

u2=rand(n,1); %uniform deviates
v2=rand(n,1); %uniform deviates
phi=pi*(v2-0.5);

xi=gammax*(sin(alpha*phi)./cos(phi)).
*(-log(u2).*cos(phi)./cos((1-alpha)*phi)).^(1-1/alpha);

%Random walk

x=cumsum(xi');
x=[0 x];

%Epochs

t=cumsum(tau');
t=[0 t];

stairs(t,x) %plots ctrw
```

Algorithm A.10. R implementation for the Monte Carlo simulation of CTRW.

```
# Plot of a single CTRW realization

# Generation of Mittag-Leffler deviates
# See Fulger, Scalas, Germano 2008 and references therein

n <- 10000 #number of points
gammat <- 1 #scale parameter
beta <- 0.95 #ML parameter

u1 <- runif(n) #uniform deviates
v1 <- runif(n) #uniform deviates

tau <- -gammat * log(u1) * (sin(beta * pi)/tan(beta * pi * v1) -
cos(beta * pi))^(1/beta)

# Generation of symmetric alpha-stable deviates
# See Fulger, Scalas, Germano 2008 and references therein

gammax <- 1 #scale parameter
alpha <- 1.95 #Levy parameter
```

```
u2 <- runif(n)
v2 <- runif(n)
phi <- pi*(v2 - 0.5)

xi <- gammax *(sin(alpha*phi)/cos(phi))*
(-log(u2)*cos(phi)/cos((1-alpha)*phi))^(1-1/alpha)

# histogram of xi
# hist(xi)

# Random walk

x <- cumsum(xi)

# Epochs

t <- cumsum(tau)

# Stairplot

plot(t,x,type="s")
```

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