

TR\_1D\_model1\_SS\FinDiff\_1D\_FirstDeriv

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```

% TR_1D_model1_SS\FinDiff_1D_FirstDeriv.m
%
% function [FirstDerivMatrix,iflag] = ...
%   FinDiff_1D_FirstDeriv(Grid,imask,iuse_upwind,velocity);
%
% This subroutine uses the finite difference method
% to return a matrix that discretizes the first
% derivative operator on a 1-D grid using either
% upwind or central differences. The procedure is
% written to be compatible with the use of a
% non-uniform grid. Values are returned only for
% discretization at the grid points where the value
% in an integer mask vector is non-zero. A uniform
% velocity value is used to determine which one-sided
% difference formula to use for the upwind direction.
%
% INPUT :
% =====
% Grid          This data structure contains the 1D grid
%               informaion :
%               .num_pts = the total number of points
%               .z = the z-coordinates of each grid point
% imask         INT(Grid.num_pts)
%               This integer mask contains a non-zero value
%               only at the interior points at which the
%               first derivative operator is to be
%               discretized.
% iuse_upwind  INT
%               If this integer flag is non-zero, then use
%               upwind finite difference formula. Otherwise,
%               use central finite differences.
%
% OUTPUT :
% =====
% FirstDerivMatrix  REAL(num_pts,num_pts) SPARSE
%               This sparse matrix contains the discretized
%               form of the first derivative operator at
%               each of the grid points with non-zero
%               imask values
% velocity         REAL
%               This is the value of the velocity in the
%               system (assumed constant by continuity)
%               and it is used to determine the upwind
%               direction from its sign.
%
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% Massachusetts Institute of Technology

```

```
% Kenneth Beers
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% Department of Chemical Engineering
% 7/2/2001
%
% Version as of 7/23/2001
```

```
function [FirstDerivMatrix,iflag] = ...
    FinDiff_1D_FirstDeriv(Grid,imask,iuse_upwind,velocity);
```

```
iflag = 0;
```

```
func_name = 'FinDiff_1D_FirstDeriv';
```

```
% This integer flag controls what action to take in the
% case of an assertion or called routine error.
```

```
i_error = 2;
```

```
% check the input
```

```
% Grid
```

```
GridType.num_fields = 2;
```

```
% .num_pts
```

```
ifield = 1;
```

```
FieldType.name = 'num_pts';
```

```
FieldType.is_numeric = 1;
```

```
FieldType.num_rows = 1;
```

```
FieldType.num_columns = 1;
```

```
FieldType.check_real = 1;
```

```
FieldType.check_sign = 1;
```

```
FieldType.check_int = 1;
```

```
GridType.field(ifield) = FieldType;
```

```
% .z
```

```
ifield = 2;
```

```
FieldType.name = 'z';
```

```
FieldType.is_numeric = 1;
```

```
FieldType.num_rows = Grid.num_pts;
```

```
FieldType.num_columns = 1;
```

```
FieldType.check_real = 1;
```

```
FieldType.check_sign = 0;
```

```
FieldType.check_int = 0;
```

```
GridType.field(ifield) = FieldType;
```

```
% perform assertion
```

```
assert_structure(i_error,Grid,'Grid',func_name,GridType);
```

```
% imask
```

```
dim=Grid.num_pts; check_column=0;
```

```
check_real=1; check_sign=2; check_int=1;
```

```

assert_vector(i_error,imask,'imask', ...
  func_name,dim,check_real,check_sign, ...
  check_int,check_column);

% iuse_upwind
check_real=1; check_sign=2; check_int=1;
assert_scalar(i_error,iuse_upwind,'iuse_upwind', ...
  func_name,check_real,check_sign,check_int);

% velocity
check_real=1; check_sign=0; check_int=0;
assert_scalar(i_error,velocity,'velocity', ...
  func_name,check_real,check_sign,check_int);

%PDL> Set an integer flag to determine whether to
% use the central, forward, or rearward finite
% difference formula.

i_FD_central = 0;
i_FD_forward = 1;
i_FD_backward = -1;

% if use central finite differences automatically
if(iuse_upwind == 0)
  i_FD_formula = i_FD_central;

% else if use upwind finite differences
else
  if(velocity > 0)
    i_FD_formula = i_FD_backward;
  elseif(velocity < 0)
    i_FD_formula = i_FD_forward;
  else
    i_FD_formula = i_FD_central;
  end
end

%PDL> Initialize FirstDerivMatrix to all zeros

% find all points at which derivative is to be
% discretized
list_points = find(imask ~= 0);
num_eval_points = length(list_points);

max_nonzero = num_eval_points*3;
FirstDerivMatrix = spalloc(...
  Grid.num_pts,Grid.num_pts,max_nonzero);

```

```
%PDL> FOR every grid point m that has a non-zero
% integer mask value
```

```
for count=1:num_eval_points
  ipoint = list_points(count);
```

```
% find indices of left, center, and right points
i_center = ipoint;
i_left = ipoint-1;
i_right = ipoint+1;
```

```
% use case statement to check for using different
% finite difference options
```

```
switch i_FD_formula;
```

```
% PDL> IF using central differences THEN
```

```
case {i_FD_central}
```

```
% PDL> Check to ensure that the point is
% not a boundary point
```

```
if(or((ipoint == 1),(ipoint == Grid.num_pts)))
  iflag = -3;
  message = [func_name, ': ', ...
    'Central FD not allowed for end point'];
  if(i_error ~= 0)
    if(i_error > 1)
      save dump_error.mat;
    end
    error(message);
  else
    return;
  end
end
```

```
% PDL> Set denom_inv = 1 / (grid_z(m+1) - grid_z(m-1))
% Set the inverse of the denominator.
```

```
denom = Grid.z(i_right) - Grid.z(i_left);
denom_inv = 1 / denom;
```

```
% PDL> FirstDerivMatrix(m,m+1) = denom_inv
```

```
FirstDerivMatrix(i_center,i_right) = denom_inv;
```

```
% PDL> FirstDerivMatrix(m,m-1) = -denom_inv
FirstDerivMatrix(i_center,i_left) = -denom_inv;

% PDL> ELSEIF using forward differences THEN
case {i_FD_forward}

% PDL> Check to ensure that the point is not the last one
if(ipoint == Grid.num_pts)
  iflag = -3;
  message = [func_name, ': ', ...
    'Forward FD not allowed for last point'];
  if(i_error ~= 0)
    if(i_error > 1)
      save dump_error.mat;
    end
    error(message);
  else
    return;
  end
end

% PDL> Set denom_inv = 1/(grid_z(m+1)-grid_z(m))
denom = Grid.z(i_right) - Grid.z(i_center);
denom_inv = 1 / denom;

% PDL> FirstDerivMatrix(m,m+1) = denom_inv
FirstDerivMatrix(i_center,i_right) = denom_inv;

% PDL> FirstDerivMatrix(m,m) = -denom_inv
FirstDerivMatrix(i_center,i_center) = -denom_inv;

% PDL> ELSEIF using rearward differences THEN
case {i_FD_backward}

% PDL> Check to ensure that the point is not the first one
```

```

if(ipoint == 1)
  iflag = -3;
  message = [ func_name, ': ', ...
    'Backward FD not allowed for first point'];
  if(i_error ~= 0)
    if(i_error > 1)
      save dump_error.mat;
    end
    error(message);
  else
    return;
  end
end
end

```

```

% PDL> Set denom_inv = 1/(grid_z(m)-grid_z(m-1))

```

```

denom = Grid.z(i_center) - Grid.z(i_left);
denom_inv = 1 / denom;

```

```

% PDL> FirstDerivMatrix(m,m) = denom_inv

```

```

FirstDerivMatrix(i_center,i_center) = denom_inv;

```

```

% PDL> FirstDerivMatrix(m,m-1) = -denom_inv

```

```

FirstDerivMatrix(i_center,i_left) = -denom_inv;

```

```

otherwise

```

```

  iflag = -4;
  message = [func_name, ': ', ...
    'Unknown FD case (' , int2str(i_FD_formula), ...
    ') encountered'];
  if(i_error ~= 0)
    if(i_error > 1)
      save dump_error.mat;
    end
    error(message);
  else
    return;
  end
end
end

```

```

%PDL> ENDIF

```

**end** % for FOR loop

**iflag = 1;**

**return;**