A System for Interfacing MATLAB with External Software Geared Toward Automatic Differentiation

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Introduction

1. Introduction
2. Linking simulation code and MATLAB
3. AMG
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What is MATLAB?

- Matrix Laboratory – The Mathworks, Inc.
- Multipurpose, multidisciplinary, extensible, mathematical software package
- Every object is a matrix.
- Mathematical syntax – easy to learn.
- Professional plotting capabilities

An (artificial) simulation

MATLAB

+

Simulation code

```
double foo(double x) {
  return sin(x)+ x*2;
}
```

- Adding non-MATLAB codes possible
- MATLAB External Interface – MEX
- Enables the use of e.g. C/Fortran codes like MATLAB functions

Interfacing with MATLAB

```
#include <mex.h>
void mexFunction(int nlhs, mxArray *plhs[],
                 int nrhs, const mxArray *prhs[]) {
   double *x, *y;
   /* Get input argument */
   x = mxGetPr(prhs[0]);
   /* Allocate storage for output argument */
   plhs[0] = mxCreateDoubleMatrix(1, 1, mxREAL);
   y = mxGetPr(plhs[0]);
   y[0]= foo_impl(x[0]);
}
```

- 8 lines of code (w/o comments) for handling one scalar argument and one scalar result.
- Even more lines of code, when handling matrices and more than one argument or result.

Automated MEX-file generation

- **Changing the simulation code may need changes of the MEX-interface.**
- **Updating the MEX-interface manually is error-prone and tedious.**
- **The Automatic MEX-file Generator (AMG) uses a small set of directives to generate sophisticated MEX-interfaces, e.g.:**

```
y=foo(x)
-kernel {
        y[0]=foo_impl(x[0]);
}
```

AMG output

```
y=foo(x)
-kernel {
        y[0]=foo_impl(x[0]);
}
```

3 lines of code

AMG

68 lines of code (comments partially stripped)

```
double foo_impl(double);
#define  x_par   arg[0]

void  mexFunction(int nlhs, mxArray *plhs[],
                  int nrhs, const mxArray *prhs[]) {

  MatObj** arg;

  arg = (MatObj **) mxMalloc( sizeof(MatObj *) * nrhs) ;

   { int i; for(i=0;i< nrhs;++i){
       arg[i] = (MatObj *) mxMalloc( sizeof(MatObj) );
       extract_all(prhs[i],arg[i]);
    }
  }

  double* x =  arg[0]->data;
  double* y;
  y = create_matrix_fast(&plhs[0],1,1,mxDOUBLE_CLASS,
                         mxREAL);

  y[0]=foo_impl(x[0]);

  /* Free temporary buffers. */
  { int i; for(i=0; i< nrhs; ++i)
     mxFree(arg[i]);
  }
  mxFree(arg);
}
```

Automatic Differentiation (AD)

- A computer program implements a mathematical function by concatenating basic operations like: +, -, *, /, sin(), tan(), ...
- AD applies the chain rule to the concatenation of the basic operations.
- AD-Tools to transform, e.g., Fortran, C or MATLAB exist.

y= f(x,c) → AD → [g_y,y]= g_f(g_x,x,c)

- More information on: http://www.autodiff.org

AMG supported differentiation

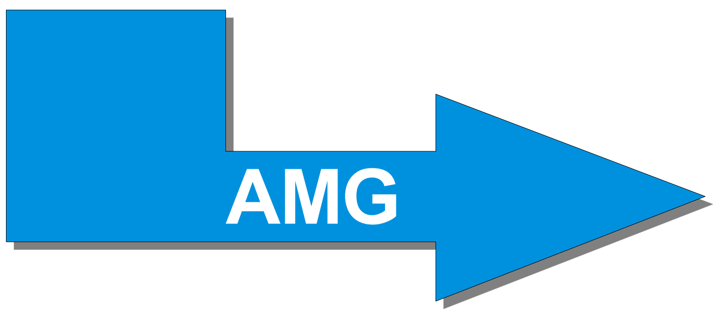
- Currently support for interfacing with two AD-tools is available:
  - ADIFOR (for Fortran77, default mode of AMG) and
  - ADiC (for C, directive `-adic` needed)
- AMG needs to know for which variables derivatives are sought (specified by the `-active()` directive).
- Conversion of data structure for Jacobian matrix:

$$\text{MATLAB} \longrightarrow \begin{cases} \text{ADiC} \\ \text{ADIFOR} \end{cases}$$

AMG-supported differentiation (2)

```
[g_y,y]=g_foo(g_x,x)
-adic
-active(x,y)
-kernel {
   ad_foo(grad(x)[0],
          grad(y)[0]);
}
```

6 lines of code

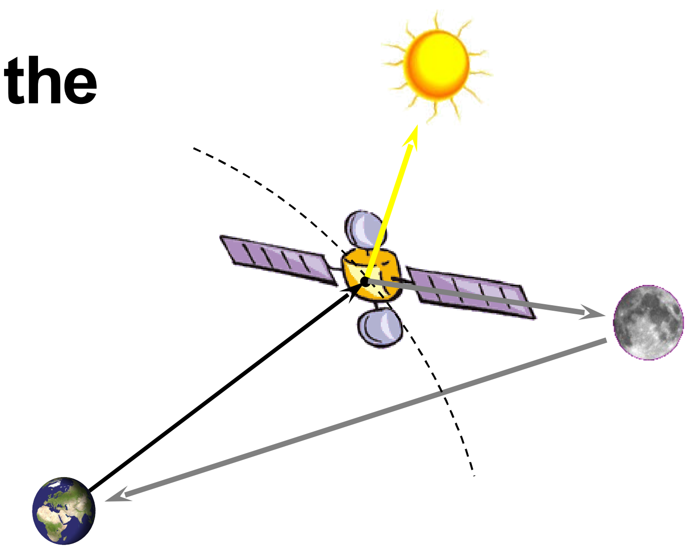


115 lines of code (comments partially stripped)

```
#define g_x_par  arg[0]
#define x_par  arg[1]

int amg_num_independents;
void mexFunction(int nlhs, mxArray *plhs[],
                 int nrhs, const mxArray *prhs[]) {

  MatObj** arg;
  arg = (MatObj **) mxMalloc( sizeof(MatObj *) * nrhs) ;

  { int i; for(i=0;i< nrhs;++i){
      arg[i] = (MatObj *) mxMalloc( sizeof(MatObj) );
      extract_all(prhs[i],arg[i]);
    }
  }

  amg_num_independents = numel(g_x) / numel(x);
  double* g_x = arg[0]->data;
  double* x = arg[1]->data;
  int* amg_itmp;
  amg_itmp = (int *) malloc(sizeof(int) * 2);
  amg_itmp[0] = numel(x) * amg_num_independents;
  amg_itmp[1] = 1;
  if(!has_equal_size(g_x_par,amg_itmp,2))
    printf("??? Error: argument 1 is not of admissible size\n");

  double* g_y;
  g_y = create_matrix_fast(&plhs[0],1 * 1 * amg_num_independents,1,mxDOUBLE_CLASS,mxREAL);
  double* y;
  y = create_matrix_fast(&plhs[1],1,1,mxDOUBLE_CLASS,mxREAL);

  ad_AD_Init(amg_num_independents);

  DERIV_TYPE* grad(x) = deriv(x,g_x);
  DERIV_TYPE* grad(y) = (DERIV_TYPE *) mxMalloc( sizeof(DERIV_TYPE) * 1 * 1);

  ad_foo(grad(x)[0], grad(y)[0]);

  get_value(grad(y),1 * 1,y);
  get_grad(grad(y),1 * 1,amg_num_independents,g_y);

  ad_AD_Final();

  /* Free temporary buffers. */
  { int i; for(i=0; i< nrhs; ++i)
    mxFree(arg[i]);
  }
  mxFree(arg);
}
```

A real life example: MSIS-86

- **MSIS-86 is a atmospheric chemistry code written by NASA in Fortran77**
- **Computes the concentrations of certain species in the atmosphere**
- **Used in a model to compute the trajectory of a satellite implemented in MATLAB**



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MSIS-86 + MATLAB

- **Called from MATLAB:**
```
[D,T] = msis86(iday, ut, alt, xlat, xlong,
                  xlst, f107a, f107, ap, mass)
```
- **A Kalman filter is applied to the trajectory of the satellite.**
- **The Kalman filter needs the derivative of `msis86()`'s `D` with respect to four inputs.**
- **AMG is used to semi-automatically generate the interface to link the two differentiated codes.**

AMG directives: AD(msis86)

```
[g_D,D,g_T,T] = g_msis_f(iday, ut, g_alt, alt, g_xlat, xlat,
       g_xlong, xlong, xlst, f107a, f107, ap, mass)

-kernel {
   int tmass = (int) mass[0];
   int tiday = (int) iday[0];
   int g_p = numel(g_alt);

   g_msis_(&g_p, &tiday, ut, alt, g_alt, xlat, g_xlat,
       xlong, g_xlong, xlst, f107a, f107, ap, &tmass,
       D, g_D, T, g_T);
}
```

MEX-Interface (1)

```
/***************************************************************
 *  AMG version 0.0.4.1av, Copyright (C) 2005 Atya El-Shekh **
 *   patched by Andre Vehreschild 2006                      **
 *                                                          **
 *    AMG is distributed under GNU General Public License   **
 ***************************************************************/


#include <stdio.h>
#include <mex.h>
#include "amgmex.h"

/**
 * The input parameters. Given an input argument arg
 * The fields of the input arguments can be accessed as follows :
 * size(arg)    : an array of integers representing the dimensions
 * ndims(arg)   : the number of dimensions
 * nrows(arg)   : the number of rows
 * ncols(arg)   : the number of columns
 * numel(arg)   : the number of the elements
 * class(arg)   : the type of the matrix object
 *
 * for cell arrays, similar macros can be used to manipulate
 * the fields.
 * celldata(arg) : a pointer to the data field of the cell array arg.
 * similarly:
 *  celldims, cellndims, cellnrows, cellncols, cellnelem, cellcalss
 **/
```

MEX-Interface (2)

```
extern void g_msis_(int*, int*, double*, double*, double*, int*,
                    double*, double*, int*, double*, double*, int*,
                    double*, double*, double*, double*, int*,
                    double*, double*, int*, double*, double*, int*);

#define  iday_par   arg[0]
#define  ut_par   arg[1]
#define  g_alt_par   arg[2]
#define  alt_par   arg[3]
#define  g_xlat_par   arg[4]
#define  xlat_par   arg[5]
#define  g_xlong_par   arg[6]
#define  xlong_par   arg[7]
#define  xlst_par   arg[8]
#define  f107a_par   arg[9]
#define  f107_par   arg[10]
#define  ap_par   arg[11]
#define  mass_par   arg[12]

int* amg_tmp;
void  mexFunction(int nlhs, mxArray *plhs[],
                  int nrhs, const mxArray *prhs[]) {

          MatObj** arg;
          void** out;
```

MEX-Interface (3)

```
  arg = (MatObj **) mxMalloc( sizeof(MatObj *) * nrhs) ;

{ int i; for(i=0;i< nrhs;++i){
            arg[i] = (MatObj *) mxMalloc( sizeof(MatObj) );
            extract_all(prhs[i],arg[i]);
  }
}


  double*        iday =  arg[0]->data;
  double*          ut =  arg[1]->data;
  double*       g_alt =  arg[2]->data;
  double*         alt =  arg[3]->data;
  double*      g_xlat =  arg[4]->data;
  double*        xlat =  arg[5]->data;
  double*     g_xlong =  arg[6]->data;
  double*       xlong =  arg[7]->data;
  double*        xlst =  arg[8]->data;
  double*       f107a =  arg[9]->data;
  double*        f107 =  arg[10]->data;
  double*          ap =  arg[11]->data;
  double*        mass =  arg[12]->data;
  int* amg_itmp;

  double* g_D;
  g_D = create_matrix_fast(&plhs[0],numel(g_alt),8,mxDOUBLE_CLASS,mxREAL);
```

MEX-Interface (4)

```
        double* D;
        D = create_matrix_fast(&plhs[1],1,8,mxDOUBLE_CLASS,mxREAL);

        double* g_T;
        g_T = create_matrix_fast(&plhs[2],numel(g_alt),2,mxDOUBLE_CLASS,mxREAL);

        double* T;
        T = create_matrix_fast(&plhs[3],1,2,mxDOUBLE_CLASS,mxREAL);


   int tmass = (int) mass[0];
   int tiday = (int) iday[0];
   int g_p = numel(g_alt);

   g_msis_(&g_p, &tiday, ut, alt, g_alt, xlat,
                            g_xlat, xlong, g_xlong, xlst, f107a, f107, ap,
                            &tmass, D, g_D, T, g_T);

        /* Free temporary buffers. */
        {
                  int i; for(i=0; i< nrhs; ++i)
                  mxFree(arg[i]);
        }
        mxFree(arg);

}
```

Conclusion

- **Benefits of AMG:**
  - **simplifies generation of MEX-interfaces**
  - **tedious and error-prone job of manually writing a MEX-interface is eased by a simple but powerful macro language**
  - **support for linking of different AD-tools**

Thank you!

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