

```
# Makefile for LMM example
#
# Daniel R. Reynolds
# Math 6321 @ SMU
# Fall 2016

CXX      = g++
CXXFLAGS = -O --std=c++11
#CXXFLAGS = -O0 -g --std=c++11

HEADERS = lmm.hpp matrix.hpp trapezoidal.hpp newton.hpp resid.hpp rhs.hpp

# executable targets
all : prob3.exe

prob3.exe : prob3.o trapezoidal.o lmm.o newton.o matrix.o
    $(CXX) $(CXXFLAGS) -o $@ $^

%.o : %.cpp $(HEADERS)
    $(CXX) -c $(CXXFLAGS) $< -o $@

# utilities
clean :
    \rm -rf *.txt *.o *.exe *
```



```
/* Linear multistep time stepper class header file. Unaltered from Dan  
* Reynolds' original file.
```

```
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```



```
#ifndef LMM_DEFINED__  
#define LMM_DEFINED__
```

```
// Inclusions  
#include <vector>  
#include <math.h>  
#include "matrix.hpp"  
#include "rhs.hpp"  
#include "resid.hpp"  
#include "newton.hpp"
```

```
// Linear multistep residual function class -- implements a  
// LMM-specific ResidualFunction to be supplied to the Newton solver.  
class LMMResid: public ResidualFunction {  
public:
```

```
    // data required to evaluate LMM nonlinear residual  
    RHSFunction *frhs;          // pointer to ODE RHS function  
    double t;                   // current time  
    double h;                   // current step size  
    Matrix yold;                // matrix of old solution vectors  
    Matrix fold;                // matrix of old right-hand side vectors  
    std::vector<double> a;       // vector of LMM "a" coefficients  
    std::vector<double> b;       // vector of LMM "b" coefficients
```

```
    // constructor (sets RHS function and old solution vector pointers)  
    LMMResid(RHSFunction& frhs_, std::vector<double> y,  
             std::vector<double> &a_, std::vector<double>& b_) {  
        frhs = &frhs_;          // set RHSFunction pointer  
        a = a_; b = b_;          // copy LMM coefficients  
        yold = Matrix(y.size(), a.size()); // allocate LMM arrays  
        fold = Matrix(y.size(), a.size());  
    };
```

```
    // initializer (fills initial set of 'old' vectors)  
    int Initialize(double t, double h, Matrix& y);
```

```
    // residual evaluation routine  
    int Evaluate(std::vector<double>& y, std::vector<double>& resid);
```

```
    // updater (shifts 'old' vectors, adding new one)  
    int Update(double t, std::vector<double>& ynew);
```

```
};
```

```
// Linear multistep residual Jacobian function class -- implements  
// a LMM-specific ResidualJacobian to be supplied to the Newton solver.  
class LMMResidJac: public ResidualJacobian {  
public:
```

```
    // data required to evaluate LMM residual Jacobian  
    RHSJacobian *Jrhs;          // ODE RHS Jacobian function pointer  
    double t;                   // current time  
    double h;                   // current step size  
    double beta;                // b_{-1} coefficient
```

```
// constructor (sets RHS Jacobian function pointer)
LMMResidJac(RHSJacobian& Jrhs_, double beta_) {
    Jrhs = &Jrhs_;    // set RHSJacobian pointer
    beta = beta_;      // copy b_{-1} coefficient
};

// Residual Jacobian evaluation routine
int Evaluate(std::vector<double>& y, Matrix& J);
};

// LMM time stepper class
class LMMStepper {

private:

    // private reusable local data
    RHSFunction *frhs;      // pointer to ODE RHS function
    LMMResid *resid;        // pointer to LMM residual function
    LMMResidJac *residJac;  // pointer to LMM residual Jacobian function
    std::vector<double> a;  // LMM coefficients
    std::vector<double> b;

public:

    NewtonSolver *newt;     // Newton nonlinear solver pointer

    // constructor (constructs residual, Jacobian, and copies y for local data)
    LMMStepper(RHSFunction& frhs_, RHSJacobian& Jrhs_, std::vector<double>& y,
               std::vector<double>& a_, std::vector<double>& b_);

    // destructor (frees local data)
    ~LMMStepper() {
        delete newt;
        delete resid;
        delete residJac;
    };

    // Evolve routine (evolves the solution via LMM)
    std::vector<double> Evolve(std::vector<double>& tspan, double h, Matrix& y);
};

#endif
```

```
/* Linear multistep time stepper class implementation file.

Class to perform time evolution of the IVP
 $y' = f(t,y)$ ,  $t$  in  $[t_0, T_f]$ ,  $y(t_0) = y_0$ 
using a linear multistep time stepping method. Although this
class is written to directly support implicit LMM, it will work
equally well for explicit LMM. Also, the initial condition fed
in to Newton solver is found using a step of explicit forward Euler.
Based off of Dan Reynolds lmm.cpp, which was just slightly altered.

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#include "lmm.hpp"

////////// LMM Residual //////////

// residual initialization routine
int LMMResid::Initialize(double t, double h, Matrix &y) {

    // copy y into stored yold object
    int ierr = yold.Copy(y);
    if (ierr != 0) {
        std::cerr << "Error in LMMResid::Initialize Copy call = " << ierr << "\n";
        return ierr;
    }

    // fill initial set of 'old' RHS vectors
    for (int j=0; j<y.Columns(); j++) {
        ierr = frhs->Evaluate(t-j*h, yold[j], fold[j]);
        if (ierr != 0) {
            std::cerr << "Error in LMMResid::Initialzie ODE RHS Evaluate call = " << ierr <<
"\n";
            return ierr;
        }
    }

    // return success
    return 0;
}

// residual evaluation routine
int LMMResid::Evaluate(std::vector<double>& y, std::vector<double>& resid) {

    // evaluate RHS function at new time (store in resid)
    int ierr = frhs->Evaluate(t+h, y, resid);
    if (ierr != 0) {
        std::cerr << "Error in ODE RHS function = " << ierr << "\n";
        return ierr;
    }

    // combine pieces to fill residual,  $y - \sum a_j y_{n-j} - h \sum b_j f_{n-j}$ 
    resid *= (-h*b[0]); // resid =  $-h*b_{-1} * f(t+h,y)$ 
    resid += y; // resid =  $y - h*b_{-1} * f(t+h,y)$ 
    for (int j=0; j<a.size(); j++)
        resid -= ( a[j] * yold[j] + (h*b[j+1]) * fold[j] );

    // return success
    return 0;
}
```

```
// Routine to handle updates of "old" solutions and right-hand sides
//
// Inputs:  tnew  the current time for the new solution
//          ynew  the new solution
// Returns: 0 (success) or 1 (failure)
int LMMResid::Update(double t, std::vector<double>& ynew) {

    // update columns of yold and fold, starting at oldest and moving to newest
    for (int icol=fold.Columns()-1; icol>0; icol--) {
        fold[icol] = fold[icol-1];
        yold[icol] = yold[icol-1];
    }

    // fill first column of yold with ynew
    yold[0] = ynew;

    // evaluate RHS function at new time (store in first column of fold matrix)
    int ierr = frhs->Evaluate(t, ynew, fold[0]);
    if (ierr != 0) {
        std::cerr << "Error in ODE RHS function = " << ierr << "\n";
        return ierr;
    }

    return 0;
};

////////// LMM Residual Jacobian //////////

// Jacobian evaluation routine
int LMMResidJac::Evaluate(std::vector<double>& y, Matrix& J) {

    // evaluate RHS function Jacobian (store in J)
    int ierr = Jrhs->Evaluate(t+h, y, J);
    if (ierr != 0) {
        std::cerr << "Error in ODE RHS Jacobian function = " << ierr << "\n";
        return ierr;
    }
    // combine pieces to fill residual Jacobian
    J *= (-beta*h); // J = -beta*h*Jrhs
    for (int i=0; i<J.Rows(); i++) // J = I - beta*h*Jrhs
        J(i,i) += 1.0;

    // return success
    return 0;
}

////////// LMM Time Stepper //////////

// LMM construction routine (allocates local data)
//
// Inputs:  frhs_  holds the RHSFunction to use
//          Jrhs_  holds the RHSJacobian to use
//          y      holds a template solution vector (for cloning)
//          a,b    hold the LMM coefficients
LMMStepper::LMMStepper(RHSFunction& frhs_,
                      RHSJacobian& Jrhs_,
                      std::vector<double>& y,
                      std::vector<double>& a_,
                      std::vector<double>& b_) {

    // check that LMM coefficients are compatible
    if (b_.size() != a_.size()+1) {
```

```
std::cerr << "LMMStepper: Incompatible LMM coefficients; will not function!\n";
return;
}

// point at and/or copy inputs
frhs = &frhs_; // set pointer to RHSFunction
a = a_;        // copy LMM coefficient arrays
b = b_;

// construct objects for nonlinear residual and its Jacobian
resid = new LMMResid(frhs_, y, a, b);
residJac = new LMMResidJac(Jrhs_, b[0]);

// construct Newton solver object (only copies y)
// (initialize with default solver parameters; user may override)
newt = new NewtonSolver(*resid, *residJac, 1.0e-7, 1.0e-11, 100, y, false);
};

// The actual LMM time step evolution routine
//
// Inputs:  tspan holds the current time interval, [t0, tf]
//          h holds the desired time step size
//          y holds the set of initial conditions, [y(0), y(-1), ..., y(-p)]
// Outputs: y holds the computed solution and set of p previous solutions,
//          [y(tf), y(tf-h), ..., y(tf-p*h)]
//
// The return value is a row vector containing all internal
// times at which the solution was computed,
// [t0, t1, ..., tN]
std::vector<double> LMMStepper::Evolve(std::vector<double>& tspan,
                                     double h, Matrix& y) {

    // initialize output
    std::vector<double> times = {tspan[0]};

    // check for legal inputs
    if (h <= 0.0) {
        std::cerr << "Evolve: Illegal h\n";
        return times;
    }
    if (tspan[1] <= tspan[0]) {
        std::cerr << "Evolve: Illegal tspan\n";
        return times;
    }
    if (y.Columns() != a.size()) {
        std::cerr << "LMMStepper: insufficient set of initial conditions, y.Columns() = "
            << y.Columns() << " and a.size() = " << a.size() << "\n";
        return times;
    }

    // initialize residual structures
    int ierr = resid->Initialize(tspan[0], h, y);
    if (ierr != 0) {
        std::cerr << "LMMStepper::Evolve error in residual Initialize call = " << ierr << "
\n";
        return times;
    }

    std::vector<double> f = y[0]; //create a vector to hold the feval

    // compute ODE RHS
    if (frhs->Evaluate(times[0], y[0], f) != 0) {
        std::cerr << "ForwardEulerStepper: Error in ODE RHS function\n";
```

```
    return times;
}

// set vector ycur to contain one step of explicit euler
std::vector<double> ycur = y[0];

// figure out how many time steps
long int N = (tspan[1]-tspan[0])/h;
if (tspan[1] > tspan[0]+N*h) N++;

// iterate over time steps
for (int i=0; i<N; i++) {

    // last step only: update h to stop directly at final time
    if (i == N-1)
        h = tspan[1]-times[i];

    // update resid and residJac objects with information on current state
    resid->t = times[i]; // copy current time into objects
    residJac->t = times[i];
    resid->h = h; // copy current stepsize into objects
    residJac->h = h;

    ycur += h*f; // one step of forward euler per time step -> one IC per time step

    // call Newton method to solve for the updated solution
    // (initial guess is one step of forward euler)
    int nerr = newt->Solve(ycur);
    if (nerr != 0) {
        std::cerr << "LMMStepper: Error in Newton solver function = " << nerr << "\n";
        return times;
    }

    // update current time (store in output array), and "old" data
    times.push_back(times[i] + h);
    resid->Update(times[i+1], ycur);
}

// copy yold data back into y Matrix
y.Copy(resid->yold);

return times;
}
```

```
/* Main routine to test a set of LMM on the scalar-valued ODE problem
   y' = lambda*y + 1/(1+t^2) - lambda*arctan(t), t in [0,3],
   y(0) = 0,
   using the O(h^3) AM and BDF time steppers.
   Based off of Dan Reynolds' LMM driver.

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#include <iostream>
#include <vector>
#include "matrix.hpp"
#include "rhs.hpp"
#include "trapezoidal.hpp"
#include "lmm.hpp"

using namespace std;

// Define classes to compute the ODE RHS function and its Jacobian

// ODE RHS function class -- instantiates a RHSFunction
class MyRHS: public RHSFunction {
public:
    double lambda; // stores some local data
    int Evaluate(double t, vector<double>& y, vector<double>& f) { // evaluates the RHS function, f(t,y)
        f[0] = lambda*y[0] + (1/(1+t*t)) - lambda*atan(t);
        return 0;
    }
};

// ODE RHS Jacobian function class -- instantiates a RHSJacobian
class MyJac: public RHSJacobian {
public:
    double lambda; // stores some local data
    int Evaluate(double t, vector<double>& y, Matrix& J) { // evaluates the RHS Jacobian, J(t,y)
        J = 0.0;
        J(0,0) = lambda;
        return 0;
    }
};

// Convenience function for analytical solution
vector<double> ytrue(const double t) {
    vector<double> yt = {atan(t)}; // via wolframalpha
    return yt;
};

// main routine
int main() {

    // time steps to try
    vector<double> h = {0.1, 0.01, 0.001, 0.0001};

    // lambda value
    vector<double> lambda = {-10.0, -100.0, -1000.0, -10000.0};
```



```
// set problem information
vector<double> y0 = {0.0};
long int M=1;
double t0 = 0.0;
double Tf = 3.0;
double dtout = 0.3;

vector<double> errs(h.size());

for (int il = 0; il<lambda.size(); il++){

    // create ODE RHS and Jacobian objects, store lambda value for this test
    MyRHS rhs;
    MyJac Jac;
    rhs.lambda = lambda[il];
    Jac.lambda = lambda[il];

    cout << "\nlambda = " << lambda[il] << ":" << endl;

    //////////// AM-2 ////////////
    // Third order Adams Moulton Method
    cout << "\n AM-2:\n";

    // create Trapezoid and LMM methods, set solver parameters
    TrapezoidalStepper TrapAM2(rhs, Jac, y0);
    vector<double> AM2_a = {1.0, 0.0};
    vector<double> AM2_b = {5.0/12.0, 8.0/12.0, -1.0/12.0};
    LMMStepper AM2(rhs, Jac, y0, AM2_a, AM2_b);
    TrapAM2.newt->SetTolerances(1.e-9, 1.e-11);
    TrapAM2.newt->SetMaxit(20);
    AM2.newt->SetTolerances(1.e-9, 1.e-11);
    AM2.newt->SetMaxit(20);

    // loop over time step sizes
    for (int ih=0; ih<h.size(); ih++) {
        cout << "  h = " << h[ih];

        // set the initial time, first output time
        double tcur = t0;
        double tout = t0 + dtout;

        // reset maxerr
        double maxerr = 0.0;

        // AM-2 requires two initial conditions
        Matrix y_AM2(M,2);
        // first is just y0 (insert into 2nd column of y_AM2)
        y_AM2[1] = y0;
        // second comes from trapezoid step step (insert into 1st column of y_AM2)
        vector<double> tspan = {tcur, tcur+h[ih]};
        y_AM2[0] = y0;
        vector<double> tvals = TrapAM2.Evolve(tspan, h[ih], y_AM2[0]);
        // update tcur to end of initial conditions
        tcur += h[ih];

        // loop over output step sizes: call solver and output error
        while (tcur < 0.99999*Tf) {

            // set the time interval for this solve
            tspan = {tcur, tout};

            // call the solver, update current time
            tvals = AM2.Evolve(tspan, h[ih], y_AM2);
            tcur = tvals.back(); // last entry in tvals
```



```
// compute the error at tcur, output to screen and accumulate maximum
vector<double> yerr = y_AM2[0] - ytrue(tcur); // computed solution is in 1st
column of y_AM2
double err = InfNorm(yerr);
maxerr = std::max(maxerr, err);

// update output time for next solve
tout = std::min(tcur + dtout, Tf);

}

cout << "\t Max error = " << maxerr;
errs[ih] = maxerr;
//convergence print out
if (ih > 0)
    cout << "\t conv rate = " << (log(errs[ih])-log(errs[ih-1]))/(log(h[ih])-log(h[
ih-1])));
    cout << endl;

}

////////// BDF-3 //////////
// Third order BDF method
cout << "\n BDF-3:\n";

// create Trapezoid and LMM methods, set solver parameters
TrapezoidalStepper TrapBDF(rhs, Jac, y0);
vector<double> BDF3_a = {18.0/11.0, -9.0/11.0, 2.0/11.0};
vector<double> BDF3_b = {6.0/11.0, 0.0, 0.0, 0.0};
LMMStepper BDF3(rhs, Jac, y0, BDF3_a, BDF3_b);
TrapBDF.newt->SetTolerances(1.e-9, 1.e-11);
TrapBDF.newt->SetMaxit(20);
BDF3.newt->SetTolerances(1.e-9, 1.e-11);
BDF3.newt->SetMaxit(20);

// loop over time step sizes
for (int ih=0; ih<h.size(); ih++) {
    cout << "  h = " << h[ih];

    // set the initial time, first output time
    double tcur = t0;
    double tout = t0 + dtout;

    // reset maxerr
    double maxerr = 0.0;

    // BDF-3 requires three initial conditions
    Matrix y_BDF3(M,3);
    // first is just y0 (insert into 3rd column of y_BDF3)
    y_BDF3[2] = y0;
    // second comes from trapezoid step step (insert into 2nd column of y_BDF3)
    vector<double> tspan = {tcur, tcur+h[ih]};
    y_BDF3[1] = y0;
    vector<double> tvals = TrapBDF.Evolve(tspan, h[ih], y_BDF3[1]);
    // update tcur to end of initial conditions
    tcur += h[ih];
    // third comes from trapezoid step step (insert into 1st column of y_BDF3)
    tspan = {tcur, tcur+h[ih]};
    y_BDF3[0] = y_BDF3[1];
    tvals = TrapBDF.Evolve(tspan, h[ih], y_BDF3[0]);
    // update tcur to end of initial conditions
    tcur += h[ih];
```

```
// loop over output step sizes: call solver and output error
while (tcur < 0.99999*Tf) {

    // set the time interval for this solve
    tspan = {tcur, tout};

    // call the solver, update current time
    tvals = BDF3.Evolve(tspan, h[ih], y_BDF3);
    tcur = tvals.back(); // last entry in tvals

    // compute the error at tcur, output to screen and accumulate maximum
    vector<double> yerr = y_BDF3[0] - ytrue(tcur); // computed solution is in 1st
column of y_BDF3
    double err = InfNorm(yerr);
    maxerr = std::max(maxerr, err);

    // update output time for next solve
    tout = std::min(tcur + dtout, Tf);

}

cout << "\t Max error = " << maxerr;

errs[ih] = maxerr;
//convergence print out
if (ih > 0)
    cout << "\t conv rate = " << (log(errs[ih])-log(errs[ih-1]))/(log(h[ih])-log(h
[ih-1]));
    cout << endl;

}
}
return 0;
}
```