PECOS

Predictive Engineering and Computational Sciences

Software Verification Workshop

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Workshop

This talk is online:

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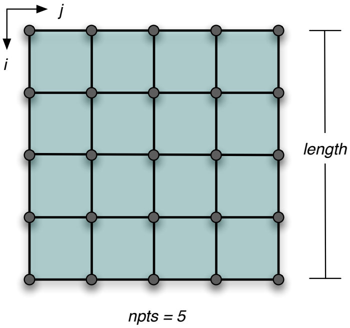
Goals

- Walk you through the process of code verification
- Build/install MASA
- Do a grid-refinement study for solution verification
- Write some code to have a little fun - do something simple and use MASA

Problem: Solve 2D Laplacian using Finite-Differencing



Recall:

- Laplace's Equation in 2D:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

- For the verification exercise, we will replace the RHS above with a forcing function $f(x, y)$ that we get from MASA

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f(x, y)$$

Problem: Solve 2D Laplacian using Finite-Differencing

Outline

- *Goal:* Write a program in C/C++, F90, or Matlab/Octave which solves the two-dimensional Laplacian on a square domain
- *Inputs*:
  - # of points in one direction (*npts*)
  - the physical dimension of one side (*length*)
- *Output*: l_2 error between your numerical solution and an exact solution derived from a manufactured solution in MASA

$$l_2 = \sqrt{\frac{\sum_{i=1}^{\mathrm{N}} (\phi_i - \phi_i^{\text{exact}})^2}{N}}$$

- *Runs*: Run your snazzy code for npts $= 5, 9, 17, and 33$ and plot l_2 norm as a function of $1/h$ where $h = length/(npts - 1)$

Finite-difference Scheme

Method

- Let us use a simple FD approximation for the Laplacian
- Assume a constant spacing mesh for convenience
- Central-differencing

$$\nabla^2 \phi_{i,j} \approx \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{h^2} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{h^2} + O(h^2)$$

- Use this formula to build the coefficient entries into a linear system $Ax = b$.
- The size of the linear system is the number of solution points. Since we are on a square domain, $N = npts * npts$
- You may find it convenient to use a mapping from a 2D index $\phi_{i,j}$ to a 1D index for the solution vector of your linear system, ϕ_{index}

$$index = j + (i * npts);$$

Finite-difference Scheme

Boundary Conditions

- The 5-point FD stencil is incomplete on the boundaries of our square domain
- We need to apply constraints to matrix A to enforce the Dirchlet conditions on the boundaries
- Simplest method to enforce BCs:
  - zero out all matrix entries on the row associated with boundary point, ϕ_i
  - set the diagonal $A(i,i)$ = 1.0
  - Set the RHS function to the desired solution $f_i = \phi_{\text{exact}}$

Finite-difference Scheme

Boundary Conditions

- Let's look at form of system matrix A^* after BCs have been applied for $npts = 3$ (note $A = \frac{1}{h^2} A^*$):

	j = 0	1	2	3	4	5	6	7	8
i = 0:	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
i = 1:	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
i = 2:	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
i = 3:	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
i = 4:	0.00	1.00	0.00	1.00	-4.00	1.00	0.00	1.00	0.00
i = 5:	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
i = 6:	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
i = 7:	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00
i = 8:	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00

- In this case, we only have *one* active interior solution point

Fortran 90 Reminder: What you need from MASA

```
program main
  use masa
  implicit none

  dx = real(lx)/real(nx)
  dy = real(ly)/real(ny);

  ! initialize the problem
  call masa_init("laplace example","laplace_2d")

  ! evaluate source terms (2D)
  do i=0, nx
     do j=0, ny

        y = j*dy
        x = i*dx

        ! evalulate source term
        field = masa_eval_2d_source_f   (x,y)

        ! evaluate analytical term
        exact_phi = masa_eval_2d_exact_phi (x,y)

     enddo
  enddo

end program main
```

C Reminder: What you need from MASA

```
#include <masa.h>

int main()
{
  err += masa_init("laplace example","laplace_2d");

  // grab / set parameter values
  Lx = masa_get_param("Lx");
  masa_set_param("Ly",42.0);

  for(int i=0;i<nx;i++)
    for(int j=0;j<nx;j++)
      {
        x=i*dx;
        y=j*dy;

        // source term
        ffield    = masa_eval_2d_source_f (x,y);

        // manufactured solution
        phi_field = masa_eval_2d_exact_phi(x,y);

       } // finished iterating over space
} //end program
```

Installing MASA locally

Steps for Building MASA:

- Grab latest tarball (https://red.ices.utexas.edu/attachments/download/1560/masa-0.40.2.tar.gz)
  - https://red.ices.utexas.edu/projects/software/files
- Untar: tar xvfz masa-0.40.2.tar.gz
- Configure: ./configure –prefix=$HOME/masa
- Compile: make -j 2
- Test: make check
- Install locally: make install
- To generate documenations: make docs
  - Can then point a broswer to docs/html/index.html

Linking to your installed MASA

Linking against your local build

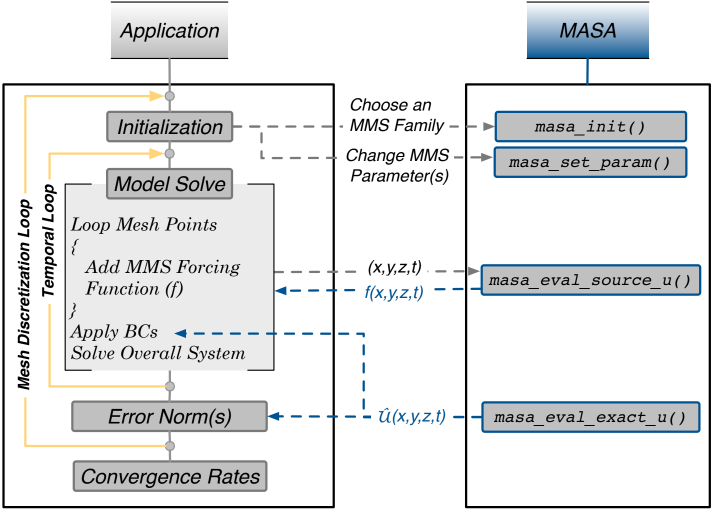
- **C**: Assuming your code is named laplacian.c and you installed masa into $HOME/masa:

```
gcc -I$HOME/masa/include laplacian.c -L$HOME/masa/lib -lmasa
```

- **F90**: Assuming your code is named laplacian.f90

```
gfortran -I$HOME/masa/lib laplacian.f90 -L$HOME/masa/lib -lmasa -lfmasa
```

General Verification Approach Using MMS and MASA



General Program Flow (a C example)

```
int main(int argc, char *argv[])
{
  int n;
  double length;
  pstruct model;                /* primary model data structure */

  /* Parse command-line */

  if(argc < 2)
    {
      printf("\nUsage: laplacian [num_pts] [length]\n\n");
      printf("where \"num_pts\" is the desired number of mesh points and \n");
      printf("\"length\" is the physical length-scale dimension in one direction\n\n");

      exit(1);
    }
  else
    {
      n      = atoi(argv[1]);
      length = (double) atof(argv[2]);
    }

  /* Problem Initialization */

  problem_initialize (n,length,&model);
  assemble_matrix    (1,&model);
  init_masa          (&model);
  apply_bcs          (&model);

  .....
```

General Program Flow (a C example, continued)

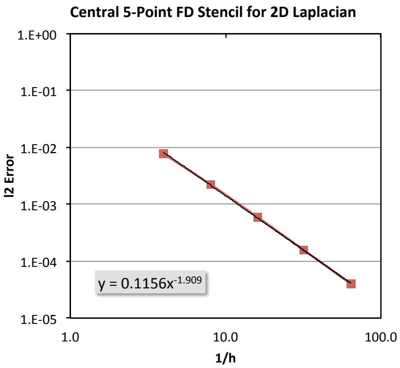
```
  /* Solve linear system */

  solve_gauss       (&model);

  /* Compute Error */

  printf("\n** Error Analysis\n");
  printf("   --> npts     = %i\n",model.npts);
  printf("   --> h        = %12.5e\n",model.h);
  printf("   --> l2 error = %12.5e\n",compute_l2_error(&model));

  return 0;

}
```

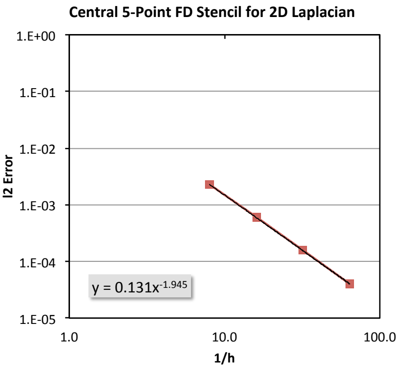
Example Model Data Structure

```
typedef struct pstruct {
  double  *phi;                  /*!< solution variable                     */
  double  *rhs;                  /*!< right-hand side forcing function      */
  double **A;                    /*!< linear system matrix                  */
  double   h;                    /*!< mesh sizing                           */
  int      n;                    /*!< problem size                          */
  int      npts;                 /*!< number of points in single direction */
  int      pad;                  /*!< pad dimension for ghost points        */
} pstruct;
```

Example Results: What we're hoping for

2nd Order Central Finite-difference Scheme





- Example results for $npts = 5, 9, 17, 33, 65$, $length = 1.0$

MASA PDE Examples

Source Terms: Euler

```
// Gas state
ADScalar T  = P / RHO / R;
ADScalar E  = 1. / (Gamma-1.) * P / RHO;
ADScalar ET = E + .5 * U.dot(U);

// Mass, momentum and energy
Scalar   Q_rho   = raw_value(divergence(RHO*U));
RawArray Q_rho_u = raw_value(divergence(RHO*U.outerproduct(U)) +
                   P.derivatives());
 Scalar  Q_rho_e = raw_value(divergence((RHO*ET+P)*U));
```

check out tests/ad_euler.cpp

Thank you for your attention.

Let’s start coding!!!