Lecture 8
Scientific Computing:
Symbolic Math, Parallel Computing, ODEs/PDEs

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CME 292
Advanced MATLAB for Scientific Computing
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Outline

Overview

- Symbolic computations in MATLAB
  - Symbolic variables, expressions, functions
- Mathematics
  - Equation solving, formula simplification, calculus, linear algebra
- Graphics
- Code generation (C, Fortran, Latex)

Symbolic variables, expressions, functions

- Create variables, expressions, functions with `sym`, `syms` commands

```
>> % Symbolic variables
>> syms x, y, z
>> % Symbolic expression
>> phi1 = sym('(1+sqrt(5))/2')
>> phi2 = sym('(1-sqrt(5))/2')
>> phi1*phi2
ans =
-(5^(1/2)/2 - 1/2)*(5^(1/2)/2 + 1/2)
>> simplify(phi1*phi2)
ans =
-1
>> % Symbolic function
>> syms f(u,v)
```

Symbolic matrices

- Symbolic matrices can be constructed from symbolic variables

```
>> syms a b c d
>> A = [a^2, b, c; d*b,c-a,sqrt(b)]
A =
[ a^2,      b,         c]
[ b*d, c - a, b^(1/2)]
>> b = [a;b;c];
>> A*b
ans =
                    a^3 + b^2 + c^2
 b^(1/2)*c - b*(a - c) + a*b*d
```

Arithmetic, Relational, and Logical Operations

- Symbolic arithmetic operations
  - `ceil`, `cong`, `cumprod`, `cumsum`, `fix`, `floor`, `frac`, `imag`, `minus`, `mod`, `plus`, `quorem`, `real`, `round`
- Symbolic relational operations
  - `eq`, `ge`, `gt`, `le`, `lt`, `ne`, `isequaln`
- Symbolic logical operations
  - `and`, `not`, `or`, `xor`, `all`, `any`, `isequaln`, `isfinite`, `isinf`, `isnan`, `logical`

http://www.mathworks.com/help/symbolic/operators.html

Equation Solving

Command	Description
`finverse`	Functional inverse
`linsolve`	Solve linear system of equations
`poles`	Poles of expression/function
`solve`	Equation/System of equations solver
`dsolve`	ODE solver

Formula Manipulation and Simplification

Command	Description
`simplify`	Algebraic simplification
`simplifyFraction`	Symbolic simplification of fractions
`subexpr`	Rewrite symbolic expression in terms of common subexpression
`subs`	Symbolic substitution

Calculus

Command	Description
`diff`	Differentiate symbolic
`int`	Definite and indefinite integrals
`rsums`	Riemann sums
`curl`	Curl of vector field
`divergence`	Divergence of vector field
`gradient`	Gradient vector of scalar function
`hessian`	Hessian matrix of scalar function
`jacobian`	Jacobian matrix
`laplacian`	Laplacian of scalar function

Calculus

Command	Description
`potential`	Potential of vector field
`vectorPotential`	Vector potential of vector field
`taylor`	Taylor series expansion
`limit`	Compute limit of symbolic expression
`fourier`	Fourier transform
`ifourier`	Inverse Fourier transform
`ilaplace`	Inverse Laplace transform
`iztrans`	Inverse Z-transform
`laplace`	Laplace transform
`ztrans`	Z-transform

Linear Algebra

- Most matrix operations available for numeric arrays also available for symbolic matrices
  - `cat`, `horzcat`, `vertcat`, `diag`, `reshape`, `size`, `sort`, `tril`, `triu`, `numel`

Command	Description
`adjoint`	Adjoint of symbolic square matrix
`expm`	Matrix exponential
`sqrtm`	Matrix square root
`cond`	Condition number of symbolic matrix
`det`	Compute determinant of symbolic matrix
`norm`	Norm of matrix or vector
`colspace`	Column space of matrix

Linear Algebra

Command	Description
`null`	Form basis for null space of matrix
`rank`	Compute rank of symbolic matrix
`rref`	Compute reduced row echelon form
`eig`	Symbolic eigenvalue decomposition
`jordan`	Jordan form of symbolic matrix

Linear Algebra

Command	Description
`chol`	Symbolic Cholesky decomposition
`lu`	Symbolic LU decomposition
`qr`	Symbolic QR decomposition
`svd`	Symbolic singular value decomposition
`inv`	Compute symbolic matrix inverse
`linsolve`	Solve linear system of equations

Assumptions

Command	Description
`assume`	Set assumption on symbolic object
`assumeAlso`	Add assumption on symbolic object
`assumptions`	Show assumptions set on symbolic variable

Polynomials

Command	Description
`charpoly`	Characteristic polynomial of matrix
`coeffs`	Coefficients of polynomial
`minpoly`	Minimal polynomial of matrix
`poly2sm`	Symbolic polynomial from coefficients
`sym2poly`	Symbolic polynomial to numeric

Mathematical Functions

Command	Description
`log`, `log10`, `log2`	Logarithmic functions
`sin`, `cos` `tan`, etc	Trigonometric functions
`sinh`, `cosh` `tanh`, etc	Hyperbolic functions

- Complex numbers and operations also available in Symbolic toolbox
- Special functions
  - Dirac, Haviside, Gamma, Zeta, Airy, Bessel, Error, Hypergeometric, Whittaker functions
  - Elliptic integrals of first, second, third kinds

Precision Control

Command	Description
`digits`	Variable-precision accuracy
`double`	Convert symbolic expression to MATLAB double
`vpa`	Variable precision arithmetic

Functions

Command	Description
`ccode`	C code representation of symbolic expression
`fortran`	Fortran representation of symbolic expression
`latex`	LaTeX representation of symbolic expression
`matlabFunction`	Convert symbolic expression to function handle or file
`texlabel`	TeX representation of symbolic expression

Exercise: Method of Manufactured Solutions

- The *method of manufactured solutions* is a general method for constructing problems with *exact, known* solutions, usually for the purpose of verifying a code.
- Consider the structural equilibrium equations

$$
\begin{aligned}
\nabla \cdot \mathbf{P} + \rho_0 \mathbf{b} &= 0 \\
\mathbf{P} &= \mathbf{S} \cdot \mathbf{F}^T \\
\mathbf{S} &= \lambda \mathrm{tr}(\mathbf{E}) \mathbf{I} + 2\mu \mathbf{E} \\
\mathbf{E} &= \frac{1}{2} \left(\mathbf{F}^T \mathbf{F} - \mathbf{I} \right) \\
\mathbf{F} &= \mathbf{I} + \frac{\partial \mathbf{u}}{\partial \mathbf{X}}
\end{aligned}
$$

Exercise: Method of Manufactured Solutions

- For the displacement field, $\mathbf{u}(\mathbf{X}) = [\mathbf{X}_1\mathbf{X}_2\mathbf{X}_3, \mathbf{X}_1^2 + \mathbf{X}_2^2, \sin(\mathbf{X}_3)]^T$, compute the corresponding forcing term
- Generate code in MATLAB, C, and Fortran to compute the forcing term from above

Outline

Programming Parallel Applications

Level of control	*Required effort*
Minimal	***None***
Some	***Straightforward***
Extensive	***Involved***

Programming Parallel Applications

Level of control	*Parallel Options*
Minimal	**Support built into Toolboxes**
Some	**High-Level Programming Constructs: (e.g. parfor, batch, distributed)**
Extensive	**Low-Level Programming Constructs: (e.g. Jobs/Tasks, MPI-based)**

Parallel support built into toolboxes

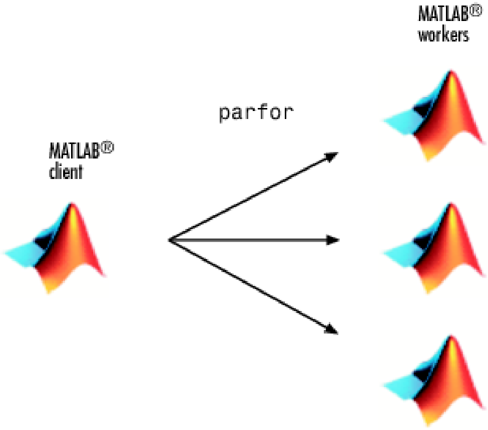
- Parallel Computations available with commands `fmincon`, `fminattain`, `fminimax`
  - Start MATLAB pool of workers
  - Set `UseParallel` option to `'always'`

```
>> matlabpool open 2
>> options = optimset('UseParallel','always');
>> x = fmincon( .., options);
```

`parfor`

- MATLAB's `parfor` opens a parallel pool of MATLAB sessions (*workers*) for executing loop iterations in parallel
- Requires loop to be embarrassingly parallel
    - Iterations must be *task* and *order independent*
        - Parameter sweeps, Monte Carlo

parfor



parfor

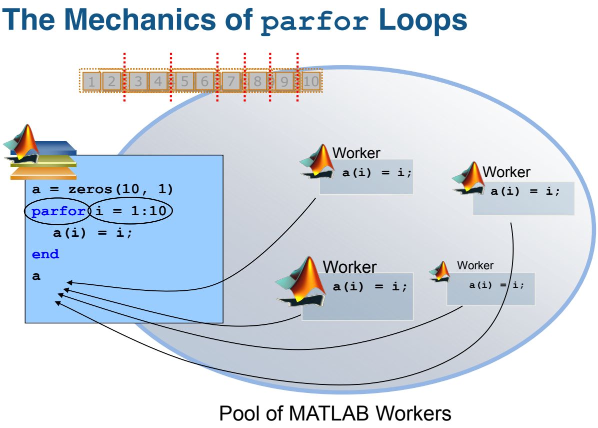


Figure : Courtesy of slides by Jamie Winter, Sarah Wait Zaranek (MathWorks)

Constraints on `parfor` body

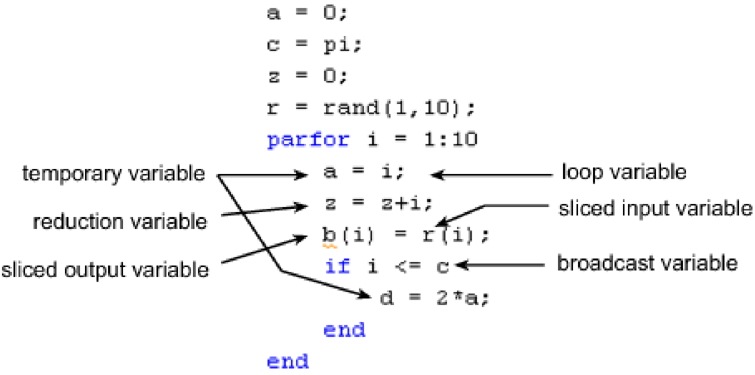
- There are constraints on the body of a `parfor` loop to enable MATLAB to automate the parallelization
  - Cannot introduce variables (`eval`, `load`, `global`, ...)
  - Cannot contain `break` or `return` statements
  - Cannot contain another `parfor` (nested `parfor` loops not allowed)

Parallel variable types

Classification	Description
`Loop`	Loop index
`Sliced`	Arrays whose segments operated on by different iterations
`Broadcast`	Variable defined outside loop (not changed inside)
`Reduction`	Accumulates value across iterations
`Temporary`	Variable created inside loop (not available outside)

`http://www.mathworks.com/help/distcomp/advanced-topics.html`

Parallel variable types



http://www.mathworks.com/help/distcomp/advanced-topics.html

Demo

`parallel_demo.m`

Outline

Introduction

- A system of *Ordinary Differential Equations* (ODEs) can be written in the form

$$\frac{\partial \mathbf{y}}{\partial t}(t) = \mathbf{F}(t, \mathbf{y})$$
$$\mathbf{y}(0) = \mathbf{y}_0$$

- The concept of *stiffness*
  - An ODE problem is stiff if the solution being sought is varying slowly, but there are nearby solutions that vary rapidly, so a numerical method must take small steps to obtain satisfactory results.
  - Numerical schemes applied to stiff problems have very restrictive time steps for stability

Numerical Solution of ODEs

- Various types/flavor of ODE solvers
  - Multi- vs single-stage
  - Multi- vs single-step
    - Number of time steps used approximate time derivative
  - Implicit vs. Explicit
    - Trade-off between ease of advancing a *single step* versus number of steps required
    - Implicit schemes usually require solving a system of equations
  - Serial vs. Parallel

Fourth-Order Explicit Runge-Kutta (ERK4)

- Multi-stage, single-step, explicit, serial ODE solver
- Consider the discretization of the time domain into $N+1$ intervals $[t_0, t_1, \ldots, t_N]$
- At step n, $\mathbf{y}_n$ is known and $\mathbf{y}_{n+1}$ is sought

$$\begin{aligned}
\mathbf{k}_1 &= \mathbf{F}(t_n, \mathbf{y}_n) \\
\mathbf{k}_2 &= \mathbf{F}(t_n + 0.5\Delta t, \mathbf{y}_n + 0.5\Delta t \mathbf{k}_1) \\
\mathbf{k}_3 &= \mathbf{F}(t_n + 0.5\Delta t, \mathbf{y}_n + 0.5\Delta t \mathbf{k}_2) \\
\mathbf{k}_4 &= \mathbf{F}(t_n + \Delta t, \mathbf{y}_n + \Delta t \mathbf{k}_3) \\
\mathbf{y}_{n+1} &= \mathbf{y}_n + \frac{\Delta t}{6}\left(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4\right)
\end{aligned} \tag{1}$$

- Fourth-order accuracy: error $= \mathcal{O}(\Delta t^4)$

Requires 4 evaluations of $\mathbf{F}$ to advance single step; does not require solving linear or nonlinear equations

Backward Euler

- Single-stage, single-step, implicit, serial ODE solver
- Consider the discretization of the time domain into $N+1$ intervals $[t_0, t_1, \ldots, t_N]$
- At step n, $\mathbf{y}_n$ is known and $\mathbf{y}_{n+1}$ is sought

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \mathbf{F}(t_{n+1}, \mathbf{y}_{n+1}) \tag{2}$$

- First-order accuracy: error $= \mathcal{O}(\Delta t)$
- A-stable

Requires solving the (nonlinear) system of equations in (2)

MATLAB ODE Solvers

- `[TOUT,YOUT] = ode_solver(ODEFUN,TSPAN,Y0)`
  - Integrates the system of differential equations $y' = f(t, y)$ from time `T0` to `TFINAL` with initial conditions `Y0`
  - `TSPAN = [T0 TFINAL]`
  - `ODEFUN` is a function handle
    - For a scalar `T` and a vector `Y`, `ODEFUN(T,Y)` must return a column vector corresponding to $f(t, y)$
  - Each row in the solution array `YOUT` corresponds to a time returned in the column vector `TOUT`
  - To obtain solutions at specific times `T0,T1,..,TFINAL` (all increasing or all decreasing), use `TSPAN = [T0 T1 .. TFINAL]`

MATLAB ODE Solvers

Command	Type	Accuracy
`ode45`	Nonstiff	Medium
`ode23`	Nonstiff	Low
`ode113`	Nonstiff	Low - High
`ode15s`	Stiff	Low - Medium
`ode23s`	Stiff	Low
`ode23t`	Moderately stiff	Low
`ode23tb`	Stiff	Low

http://www.mathworks.com/help/matlab/ref/ode45.html

Assignment

Use `ode45` and `ode23s` to solve the simplified combustion model

$$y'(t) = y^2(1-y), \qquad 0 \leq t \leq 2/\epsilon, \qquad y(0) = \epsilon$$

- Try $\epsilon = 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1$
- How many time steps were required for `ode45` for each epsilon? How many for `ode23s`?
  - `length(TOUT)` using the notation from earlier
- For $\epsilon = 10^{-4}$, plot $y(t)$

Outline

1. Symbolic Math Toolbox
    - Symbolic Computations
    - Mathematics
    - Code generation
2. Parallel Computing Toolbox
3. Ordinary Differential Equations
4. Partial Differential Equations
    - Overview
    - Mesh Generation in MATLAB
    - PDE Toolbox
5. Conclusion

Motivation

- Partial Differential Equations are ubiquitous in science and engineering
    - Fluid Mechanics
        - Euler equations, Navier-Stokes equations
    - Solid Mechanics
        - Structural dynamics
    - Electrodynamics
        - Maxwell equations
    - Quantum Mechanics
        - Schrödinger equation
- Analytical solutions over arbitrary domains mostly unavailable
- In some cases, existence and uniqueness not guaranteed

Numerical Solution of PDEs

- Classes of PDEs
  - Elliptic
  - Parabolic
  - Hyperbolic
- Numerical Methods for solving PDEs
  - Finite Difference (FD)
  - Finite Element (FE)
  - Finite Volume (FV)
  - Spectral (Fourier, Chebyshev)
  - Discontinuous Galerkin (DG)

Numerical Solution of PDEs

The (major) steps required to compute the numerical solution of to a system of Partial Differential Equations are

- Derive discretization of governing equations
  - Semi-discretization
  - Space-time discretization
  - Boundary conditions
- Construct spatial mesh (or space-time mesh)
  - Structured vs. Unstructured
    - Codes can be written to leverage structured mesh
    - Unstructured meshes more general
  - Requirements on mesh heavily depend on application of interest and code used
- If semi-discretized, define temporal mesh
- Implement and solve
- Postprocess

Example: Semi-Discretization

Consider the *viscous* Burger's equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \epsilon \frac{\partial^2 u}{\partial x^2} \tag{3}$$

for $x \in [0, 1]$, with the initial condition $u(x, 0) = 1$ and boundary condition $u(0, t) = 5$.

Spatial discretization of (3) yields a system of ODEs of the form

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{F}(\mathbf{U}(t), t), \tag{4}$$

this is known as *semi-discretization* or the *method of lines*.

Example: Mesh

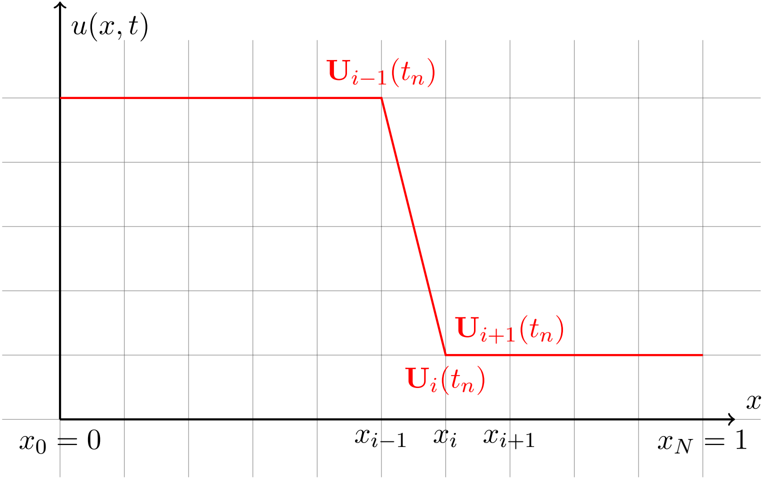


Figure : Discretized domain and solution for (3)

Example: Finite Difference Method

- We approximate the first-order derivative with a *backward* difference on the previous grid to objtain

$$\frac{\partial u}{\partial x}(x_i, t) \approx \frac{u(x_i, t) - u(x_{i-1}, t)}{\Delta x} \tag{5}$$

for $i = 1, \ldots, N$ where $\Delta x_i = x_i - x_{i-1} = \Delta x$ as the grid is assumed uniform.

- The standard central second-order approximation to the diffusive term is applied

$$\frac{\partial^2 u}{\partial x^2}(x_i, t) \approx \frac{u(x_{i+1}, t) - 2u(x_i, t) + u(x_{i-1}, t)}{\Delta x^2} \tag{6}$$

for $i = 1, \ldots, N - 1$

Example: Finite Difference Method

- At the last equation, a first-order, leftward bias of the second-order derivative is applied

$$\frac{\partial^2 u}{\partial x^2}(x_i, t) \approx \frac{u(x_N, t) - 2u(x_{N-1}, t) + u(x_{N-2}, t)}{\Delta x^2}. \qquad (7)$$

- The boundary condition is applied as

$$u(x_0, t) = u(0, t) \qquad (8)$$

in (5) and (7).

Mesh Generation

In 1D, mesh generation is trivial. Difficulties arise in 2D and higher.

- PDE Toolbox
  - 2D only
- `distmesh`
  - Both 2D (triangles) and 3D (tetrahedra)
  - Unstructured
  - Per-Olof Persson

PDE Toolbox

- Geometry definition (points, curves, surfaces, volumes)
- Mesh generation
- Problem definition
- Solution
- Postprocessing

PDE Toolbox

- Standard MATLAB distribution
  - `pdepe` for solving initial boundary-value problems for *parabolic-elliptic* PDEs in 1D
- PDE Toolbox
  - Graphical User Interface
    - `pdeapp`
    - Demo
  - Command Line

Geometry Definition

- Construct mesh interactively using `pdetool`
  - Unions and intersections of basic shapes
    - Rectangles, ellipses, circles, etc
- Use `pdegeom` to create geometry programmatically
  - Build parametrized, oriented boundary edges
  - Label left and right regions of edges
  - Geometry built from union of regions with similar labels
  - Demo: `naca`

Mesh Generation

Command	Description
initmesh	Create initial triangular mesh
adaptmesh	Adaptive mesh generation and PDE solution
jigglemesh	Jiggle internal points of triangular mesh
reinemesh	Refine triangular mesh
tri2grid	Interpolate from PDE triangular mesh to rectangular grid
pdemesh	Plot PDE triangular mesh
pdetriq	Triangle quality measure

```
>> [p,e,t]=initmesh('naca');
>> pdemesh(p,e,t), axis equal
```

Problem Definition: PDE

- Both scalar and vector PDEs available in PDE toolbox
- Here we focus on scalar PDEs
  - Elliptic

$$-\nabla \cdot (c\nabla u) + au = f \tag{9}$$

  - Parabolic

$$d\frac{\partial u}{\partial t} - \nabla \cdot (c\nabla u) + au = f \tag{10}$$

  - Hyperbolic

$$d\frac{\partial^2 u}{\partial t^2} - \nabla \cdot (c\nabla u) + au = f \tag{11}$$

  - Eigenvalue

$$-\nabla \cdot (c\nabla u) + au = \lambda du \tag{12}$$

- PDE coefficients a, c, d, f can vary with space and time (can also depend on the solution u or the edge segment index)

Problem Definition: Boundary Conditions

- Boundary conditions available for both scalar and vector available in PDE toolbox
- Here we focus on scalar PDEs
  - Dirichlet (essential) boundary conditions

$$hu = r \text{ on } \partial\Omega \tag{13}$$

  - Generalized Neumann (natural) boundary conditions

$$\mathbf{n} \cdot (\nabla u) + qu = g \text{ on } \partial\Omega \tag{14}$$

- Boundary coefficients h, c, r, q, g can vary with space and time (can also depend on the solution u or the edge segment index)

Specify Boundary Conditions

Boundary conditions can be specified:

- Graphically using `pdetool`
- Programmatically using `pdebound`
  - `[q,g,h,r] = pdebound(p,e,u,time)`
  - Demo: `nacabound`

Specify PDE Coefficients

PDE coefficients can be specified:

- Graphically using `pdetool`
- Programmatically via constants, strings, functions
  - `u = parabolic(u0,tlist,b,p,e,t,c,a,f,d);`
    - `u0` - initial condition
    - `tlist` - time instances defining desired time steps
    - `b` - function handle to boundary condition
    - `p`, `e`, `t` - mesh
    - `c`, `a`, `f`, `d` - PDE coefficients (numeric, string, functions)

PDE solvers

- Elliptic
    - `[u,res]=pdenonlin(b,p,e,t,c,a,f);`
- Parabolic
    - `u=parabolic(u0,tlist,b,p,e,t,c,a,f,d);`
    - Demo: `workflow`
- Hyperbolic
    - `u=hyperbolic(u0,ut0,tlist,b,p,e,t,c,a,f,d);`
- Systems of Equations

Outline

Lecture 9

- Our final lecture will be this Thursday (May 1) in this room at regular time
- Optional lecture
- No homework associated with this lecture
- I will cover
  - Publication-Quality Graphics
  - Animation
  - Partial Differential Equations and PDE Toolbox

What Now?

- Classes (non-exhaustive)
  - Numerical Linear Algebra
    - EE 263, CME 200, CME 302, CME 335
  - Numerical Optimization
    - CME 304, CME 334, CME 338
  - Object-Oriented Programming
    - CS 106B, CS 108
  - ODEs/PDEs
    - CME 102, CME 204, CME 206, CME 303, CME 306
  - Additional Advanced MATLAB classes (none to my knowledge)
    - Interest in taking this class as a full quarter class (3 units)
    - Indicate in evaluations
    - Email Margot Gerritsen (margot.gerritsen@stanford.edu)
- Future MATLAB questions
  - You have my email!

Teaching Evaluations

- Very important so please complete them
- Detailed comments in evaluations regarding the pros and cons of the course will be *much* appreciated
- Not available until end of Quarter
- If you have something important you wish to convey
  - Make a note of it now so you don't forget in a month
  - Email Margot (margot.gerritsen@stanford.edu)