CE 60422 - FATE & TRANSPORT OF CONTAMINANTS IN ENVIRONMENTAL FLOWS

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Office Hours: Honestly, any time that works for you and I am free. Just stop by my office or schedule an appointment. Formally I will always be available after class on Tuesdays.

Welcome to CE 60422! I hope that this course is rewarding to you and that you develop an appreciation for how contaminants move and how we can mathematically represent that movement. This course will lean more on the theoretical side, but I will try when appropriate to bring in real data from real systems.

This is the third time I am teaching this course and I personally am always learning how to be a better teacher, so continuing feeback is **desired** and **encouraged** both in terms of how to improve course content and conveyace as well as in my personal teaching style. Lets make this a great course together. My goals for this course are broadly speaking

1. Introduce you to the basic concepts and techniques that have been classically used to study contaminant transport.
2. Introduce you to state of the art modelling techniques that better represent features often observed in real environmental systems, where classical approaches often fail.
3. Use well known situations to help you learn these concepts
4. Help you to develop skills in approaching complex problems where there may not be a single 'correct' answer or approach. Guesstimation and educated judgement are strongly encouraged and will be rewarded.
5. Encourage you to THINK, OBSERVE, and ANALYZE

The primary means by which we will work together towards these goals are:

1. Lectures: I am looking for ACTIVE participation by each of you in the learning process,
2. Assignments: Significant effort on your part in completing assignments.

As with all courses at Notre Dame, this course is covered by the Honor Code.

Requirements - I see no 'strict' requirements for this class. However there are two things you may wish to consider as they will make your life easier:

- A solid foundation in Calculus (and preferably differential equations)
- An ability to program

Not having these will not hinder you from taking this class, but it will mean a substantial effort on your part to develop and polish these skills (I am happy to provide the support you need).

With regard to programming in particular, a siginifant portion of this course will involve computer programming, as without it there is very little one can actually do, and I DO expect you to be able to do it. It is your choice what language you use to implement these codes and I do not mind what you choose as long as it works for you.

I will be working primarily with MATLAB and MATHEMATICA, both of which you should be able to download and install on your personal computers from oit.nd.edu. I expect you to do so, unless you choose a different set of equivalent languages.

Most of you I hope are familiar, at least superficially, with MATLAB. If not, please come and see me. MATLAB is a high level/ scritping language. By high level I mean that it does ot require compilation and the likes. It is not always the most efficient tool, but it is a language of choice for many people, because it is intuitive and easy to use relative to many alternatives. Given how powerful even laptops are nowadays you can solve many problems of interest both quickly, efficiently and easily in MATLAB. If you prefer to work with something you already know (e.g. C,C++,Fortran, Python,PEARL, R) feel free to do so. Indeed, most things that will be done in this class could be done wth a spreadsheet such as Excel, although I do not recommend this as the higher level concepts, while doable, become in my view excessively painful and difficult to implement (but I have seen students do it with success).

MATHEMATICA is what is called a symbolic maths programming language and can basically do mathematics for you (while you should know what Mathematica is doing and actually be able to do it yourself, it takes much of the tediousness out of it and if used correctly avoids typical sloppiness mistakes such as loss of minus signs, etc). It is an incredibly powerful tool that can solve systems of algebraic equations, differential equation, perform integration, perform mathematical transformations, plot complex systems as well as many many more things (see http://www.wolfram.com/mathematica/ for details). An alternative to Mathematica is MAPLE, which is what I typically use (but is only availabe to faculty at ND). If you can get a copy and would prefer to use it that's fine bye me. Both programs do pretty much the same thing, but some of the new tools in MATHEMATICA are pretty amazing (e.g. you can just write what you want MATHMEATICA to do without following the proper language protocal and it will make its best guess on interpreting what you have asked it to do – i.e. you don't even have to learn the details of the language properly if you do not want to).

For those of you who do not have programming experience, take advantage of this course to learn it. Programming is an invaluable skill that will be useful to you regardless of what your future holds and once you know the basics in one language learning another is straightforward.

Topics we will cover in this class

The topics listed below are approximate and subject to change. If you have suggestions or interests, LET ME KNOW and I will try to work them in!

Lecture Topics to be Covered

- The Diffusion equation - Solution methods via Fourier Transforms, Greens functions. Generalizations to arbitrary source, boundary and initial conditions.
- Brownian Motion and Random Walk Methods for simulating diffusive systems
- Advection-Diffusion and Retardation
- Taylor Dispersion (the role of heterogeneous velocity fields on large scale transport)
- First order degradation reaction systems
- Mixing Processes and Mixing Driven Reactions.
- Measures of mixing and how different mixing mechanisms affect how quickly systems dilute or how quickly reactions will occur.

The second part of the course will be directed at more sophisticated modeling techniques that aim to capture observations, commonly seen in environmental systems, but that classical models cannot capture due to assumptions inherent to those models that are being violated in real systems. Specifically I will aim to cover:

- Reactive Random Walks.
- Mobile-Immobile Models
- Fractional Dispersion Models (both fractional in space and time). This will include subdivision, superdiffusion and Levy flights. By the way fractional dispersion here means that in our governing equation we have derivatives that are not integer order i.e. d^\alpha C/d x^\alpha where 1<\alpha<2, which most people do not even know what that means.
- Continuous Time Random Walks
- Markov Chain Models

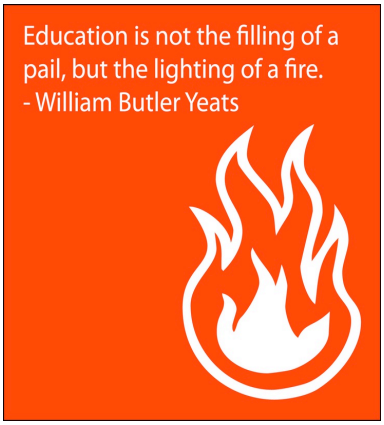
If we do not get to cover all of these I am happy to provide required information so you can learn them yourself. The ourse will move at the pace needed to ensure that those who are working hard are getting the most out of it and if that means only covering a small part of what I want to cover – so be it!

Your responsibilities

Homework (most likely weekly)

(Depending on how much effort and learning I see from you guys) Midterm and Final Exams.

Personal Statement of My Goal for this Course



The nature of this course will be very mathematical. For some of you the maths may be easy, for some of you very hard. I promise to always be there to help you with it and teach it to you in as many different ways as needed and I can, so that you will succeed! My office is always open to you – I mean it when I say that the most satisfying part of my job is to have students come and chat with me – it brightens my day (even just to chat informally) and nothing is more satisfying than seeing the switch go 'Click' when a student gets it.

I am not interested in testing your mathematical skills, nor am I really interested in testing you at all. A grad class in my view is about exposing you to new ideas and details you are not aware of and pushing the limits of your knowledge and skills. As Yeats best said I want to 'ignite a fire' in you (see quote above). If you guys step up to the challenge and work hard with and for me, a final grade should be the last thing you should worry about.

My goal is to expose you to what I think are extremely elegant and beautiful methods for understanding very complex phenomena.

Struggle with me, work hard and be patient and you will find it very rewarding as you will start to see the equations and processes everywhere you look around you (as I do and know my grad students begin to also). I expect you to work hard and put in the hours needed to learn the material, but that also means that you should expect me to work hard for you – hold me to the highest standard and expect nothing less than that from me – if I am failing you – let me know and I will do my best to rise to the occasion.

If what I am teaching is easy for you – push yourself harder and try to take these concepts a level further by implementing more elegant approaches and solutions than those I teach you – I am happy to provide more challenging and interesting problems!

Once you get these things, as hard as they may initially seem, they become 'SIMPLE' and I believe that Simplicity is the root of elegance and success in problem solving for Scientists and Engineers.