Particle dynamics class, SMS 618, Emmanuel Boss

Aggregation lab, using Matlab code compiled by George Jackson.
Source code: http://ocean.tamu.edu/%7Eecomodel/Software/coagmodel/coagintro.html

Today you will run a program that computes the effects of growth, settling and aggregation on the particulate size distribution (PDF) in a mixed layer. The code is designed to look at the interplay of growth, coagulation and sinking in determining the standing stock of phytoplankton in the mixed-layer.

The program is designed to solve:

$$\frac{dN(D,t)}{dt} = \mu N(D) + \frac{1}{2}\int_0^D \alpha(D_1, D-D_1)\beta(D_1, D-D_1)N(D_1,t)N(D-D_1,t)dD_1$$

$$-\int_0^\infty \alpha(D_1, D)\beta(D, D_1)N(D_1,t)N(D,t)dD_1 - \frac{w_s}{H_{ml}}N(D)$$

The first term on the RHS is growth and the last term is loss through sinking.
The main program is called 'simple.m' and can be run directly from the command line.

Simple.m is a script to handle all the calculations for a simple coagulation program. It calls three other scripts which may be called separately:

- simpbeta.m- a program to calculate and save the betas that describe interaction rates. It assumes a shear =1/s; this is adjusted to fit the desired problem in simpcoag.m.
- Simpcoag.m- a program to calculate the change in time of the particle size spectra. The betas only have to be changed when the one of the parameters used to calculate them changes. It is quicker to reuse previously calculated values.
- Simpgraph.m-a program to graph the output from simpcoag.m. The results of simpcoag.m are saved in the file simpout.mat. Note: I changed one line in this program to allow us to compare runs one after the other.

Each program has a standard set of parameter values that you accept in one of two ways:

1. hit a carriage return at the start of the program and accept all.
2. type in "1" and hit a cr at the start. You will then be offered the option of changing or keeping the default value of each whose value will be displayed in square brackets. You may:
   a. Accept the value by hitting the cr key
   b. Change the value by typing in the new value and hitting cr.

Inputs to simpbeta.m:

1. fr-fractal dimension [default=2.33]. Observations suggest $2<fr\leq 3$.
2. nsect-number of section in the PSD [default=10]. The higher the value the longer the computation (and the more realistic the results). The section's size increase with size.
3. dia0-minimun diameter in cm [default=0.002cm]. Sections are spaced $2^{1/3}$ diameter from each other (of 2*volume for fr=3). The bigger the number of section the bigger the size of the biggest floc.
4. delrho-'Unit particle density (g/cc)' [default= 0.036159, based on observation of settling phytoplankton]. This is the excess density, ρ_p-ρ_{fluid}, of the primary particle.
5. nkernel-type of coagulation kernel [default=3-fractal] kernel. 1-Rectilinear (does not take into account flow around particles), 2-curviliniear (takes into account flow around largest particle), and 3-fractal (takes into account fractal properties in computation of the kernel).
6. Name of output file for betas: default is betaf– can be used for many successive calculations.

Inputs to simpcoag.m:

1. cbeta— Input name of file with betas [default: betaf].
2. tfinal— Input final time (in days) [default: 20 days].
3. alpha— Input stickiness [default: 1]. Varies from 0 to 1. Aggregation kernel is proportional to alpha. No aggregation is possible if alpha=0.
4. zthick— Input layer thickness onelayer(in meter)-mixed layer depth [default=65m]. Important in determining the role of sinking; the sinking term is inversely proportional to it.
5. Lgam—Input shear (1/s) [default=0.1]. Turbulent shear level. A realistic upper bound for strongly wind driven ML is $1s^{-1}$.
6. Lmu—specific growth rate of smallest size class (1/day) [default=0.15 d^{-1}]. Phytoplankton vary in their growth rate to a maximum of about on doubling per day, or $\mu=\ln(2)\ d^{-1}$.
7. num_1— Input initial number of monomers (#/cm^3) [default=40cm^{-3}]. This is the initial concentration of the monomers. The other sections are filled in at time zero assuming an equilibrium spectrum.
8. nsecgro—Input the section at which allow growth in aggregates. [default=4, i.e. first four aggregation sections]. 0-no growth in aggregates.
9. rt—relative tolerance [Default= 3e-014]. No need to change except for evaluating whether convergence has been achieved.
10. at—absolute tolerance[Default= 1e-016]. No need to change except for evaluating whether convergence has been achieved.

Note on the program:

a. variables are in many different units.

b. you can change variables in the command line or within the programs by varying the default value and accepting the defaults when running the program.

Exercise:

1. Familiarize yourself with the program by running it with its default parameters.
2. Try to predict what will happen qualitatively (compared to the standard run, but without growth in aggregates) if you set:
    a. Phytoplankton growth-rate=0;
    b. Stickiness efficiency=0;
    c. Shear rate of $1s^{-1}$;
    d. C_0=400particles/cm^3 for initial concentration;
    e. H_{ml}=5 or 500m?
    f. Double/half the number of sections (changing the size of the biggest aggregate present).
3. Assuming a single particle size class, the equilibrium solution will have: $C_{attractor}=(\mu-w\_s/H_{ml})/\alpha\beta$. Is this consistent with what you observe as $t\rightarrow\infty$ (test by varying $(\mu-w\_s/H_{ml})/\alpha$ (for constant β)?
4. The time scale for adjustment of the size distribution when coagulation dominates over growth is $\propto 1/\{\alpha\beta C_0\}$. It is μ when growth-rate dominates (e.g. at small concentrations). Play with μ, C_0 and α (for constant β) and see whether it pertains for the complex model.
5. Experiment with changing the coagulation kernels (rectilinear, curvilinear and fractal) and see how things change.