## Particle Dynamics in the Ocean: Marine Particle Processes and their Representation

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# How do we describe particles? How do we represent particle dynamics?

#### Martin Curve



b  $\mathsf{F}(z) = \mathsf{F}_{100} \left(\frac{z}{100}\right)'$  $b = -0.973 \rightarrow -0.319$ b = -0.858

Martin et al., 1987



# Some Philosophy

- Modeling as simulation
  - Reproduce the data
  - Fit simple functions
- Modeling as theory
  - Use first principles to make predictions
  - Allow for spatial & temporal variability
- Suite of models at different scales



# Particle Size Spectra





Jackson et al., 1997



#### Southern Ocean

#### Eastern Atlantic

#### Equatorial Pacific

De La Roch & Passow, 2007 (Data from Guidi et al.)

### Variations in spectral slope





# **Coagulation Equation**

$$\frac{\mathrm{dn}(\mathbf{m}, \mathbf{t})}{\mathrm{dt}} = \frac{\alpha}{2} \int_0^m \beta(\mathbf{m}_j, \, \mathbf{m} - \mathbf{m}_j) \mathbf{n}(\mathbf{m} - \mathbf{m}_j, \, \mathbf{t}) \mathbf{n}(\mathbf{m}_j, \, \mathbf{t}) \, \mathrm{dm}_j$$
$$- \alpha \mathbf{n}(\mathbf{m}, \, \mathbf{t}) \int_0^\infty \beta(\mathbf{m}, \, \mathbf{m}_j) \mathbf{n}(\mathbf{m}_j, \, \mathbf{t}) \, \mathrm{dm}_j$$
$$- \mathbf{n}(\mathbf{m}, \, \mathbf{t}) \frac{w_s(\mathbf{m})}{z} + \mathbf{I}(\mathbf{m}, \, \mathbf{t})$$

# **Coagulation kernels**

$$\frac{\mathrm{d}n(\mathbf{m}, \mathbf{t})}{\mathrm{d}t} = \frac{\alpha}{2} \int_0^m \beta(\mathbf{m}_j, \mathbf{m} - \mathbf{m}_j) n(\mathbf{m} - \mathbf{m}_j, \mathbf{t}) n(\mathbf{m}_j, \mathbf{t}) \, \mathrm{d}\mathbf{m}_j$$
$$- \alpha n(\mathbf{m}, \mathbf{t}) \int_0^\infty \beta(\mathbf{m}, \mathbf{m}_j) n(\mathbf{m}_j, \mathbf{t}) \, \mathrm{d}\mathbf{m}_j$$
$$- n(\mathbf{m}, \mathbf{t}) \frac{w_s(\mathbf{m})}{z} + I(\mathbf{m}, \mathbf{t})$$

#### **Coagulation Mechanisms** Differential **Fluid Shear Brownian Motion** Sedimentation $\beta(\mathbf{r}_i,\mathbf{r}_j) = \pi(\mathbf{r}_i + \mathbf{r}_j)^2 |w_j - w_i|$ $\beta(\mathbf{r}_{i},\mathbf{r}_{j}) = 1.3 \left(\frac{\epsilon}{\nu}\right)^{1/2} (\mathbf{r}_{i} + \mathbf{r}_{j})^{3}$ $\beta(\mathbf{r}_{i},\mathbf{r}_{j}) = \frac{2}{3} \frac{kT}{\mu} \frac{(\mathbf{r}_{i} + \mathbf{r}_{j})^{2}}{\mathbf{r}_{i}\mathbf{r}_{j}}$ $\beta(\mathbf{r}_{i}, \mathbf{r}_{j}) = 0.5\pi \mathbf{r}_{j}^{2} |w_{j} - w_{i}|$ $\beta(r_i, r_j) = \frac{p^2}{1+2p^2} \left(\frac{\varepsilon}{\nu}\right)^{1/2} (r_i + r_j)^3$

#### **Stickiness**

$$\frac{\mathrm{dn}(\mathrm{m},\mathrm{t})}{\mathrm{dt}} = \underbrace{\bigotimes}_{2} \int_{0}^{\mathrm{m}} \beta(\mathrm{m}_{j}, \mathrm{m} - \mathrm{m}_{j}) n(\mathrm{m} - \mathrm{m}_{j}, \mathrm{t}) n(\mathrm{m}_{j}, \mathrm{t}) \mathrm{dm}_{j}$$
$$- \underbrace{\bigotimes}_{0} n(\mathrm{m}, \mathrm{t}) \int_{0}^{\infty} \beta(\mathrm{m}, \mathrm{m}_{j}) n(\mathrm{m}_{j}, \mathrm{t}) \mathrm{dm}_{j}$$
$$- n(\mathrm{m}, \mathrm{t}) \frac{w_{s}(\mathrm{m})}{z} + \mathrm{I}(\mathrm{m}, \mathrm{t})$$

Stickiness: largely biological & chemical? Transparent exopolymer particles - nanogels?

### Nanoparticles



Verdugo, Ann. Rev. Mar. Sci., 2012

### Nano-gels



Metcalfe et al., J. Coll. Int. Sci., 2006

Polymers with stickinesss varying along their length

Distribution of stickiness and polymer rigidity affects fractal dimension, gel size, aggregation times

# Settling

$$\frac{\mathrm{dn}(\mathrm{m},\mathrm{t})}{\mathrm{dt}} = \frac{\alpha}{2} \int_0^{\mathrm{m}} \beta(\mathrm{m}_j, \,\mathrm{m} - \mathrm{m}_j) n(\mathrm{m} - \mathrm{m}_j, \,\mathrm{t}) n(\mathrm{m}_j, \,\mathrm{t}) \,\mathrm{dm}_j$$
$$-\alpha n(\mathrm{m}, \,\mathrm{t}) \int_0^{\infty} \beta(\mathrm{m}, \,\mathrm{m}_j) n(\mathrm{m}_j, \,\mathrm{t}) \,\mathrm{dm}_j$$
$$-\frac{n(\mathrm{m}, \mathrm{t}) \frac{w_s(\mathrm{m})}{z}}{+} I(\mathrm{m}, \mathrm{t})$$

# **Settling Speed**



McDonnell & Buesseler, Limnol. Oceanogr., 2011



Settling Velocity Traps

♦ March-May - 200 m - SV1

∆ March-May - 200 m - SV2 □ May-July - 200 m - SV1&2

1000 =

10

Peterson et al., Limnol. Oceanogr. Methods, 2005

# Input/Growth

$$\frac{\mathrm{d}n(\mathrm{m},\mathrm{t})}{\mathrm{d}\mathrm{t}} = \frac{\alpha}{2} \int_0^{\mathrm{m}} \beta(\mathrm{m}_j, \,\mathrm{m} - \mathrm{m}_j) n(\mathrm{m} - \mathrm{m}_j, \,\mathrm{t}) n(\mathrm{m}_j, \,\mathrm{t}) \,\mathrm{d}\mathrm{m}_j$$
$$- \alpha n(\mathrm{m}, \,\mathrm{t}) \int_0^{\infty} \beta(\mathrm{m}, \,\mathrm{m}_j) n(\mathrm{m}_j, \,\mathrm{t}) \,\mathrm{d}\mathrm{m}_j$$
$$- n(\mathrm{m}, \mathrm{t}) \frac{w_s(\mathrm{m})}{z} + I(\mathrm{m}, \mathrm{t})$$





#### Mass Balance



$$\begin{aligned} & \text{Integral Models} \\ & \text{Mass concentration } \frac{d\varphi}{dt} = \mu\varphi - \frac{F_{\varphi}}{Z} \\ & \text{Number concentration } \frac{d\psi}{dt} = \mu\psi - \frac{F_{\psi}}{Z} - \xi \\ & F_{\psi} = \int_{d_0}^{\infty} w(d)n(d) \, dd \quad F_{\varphi} = \int_{d_0}^{\infty} C(d)w(d)n(d) \, dd \\ & \xi = \frac{\alpha}{2} \int_{d_0}^{\infty} \int_{d_0}^{\infty} \left(\beta_{\text{shear}}(d_1, d_2) + \beta_{\text{ds}}(d_1, d_2)\right)n(d_1)n(d_2) \, dd_1 \, dd_2 \\ & n(d) = Ad^{-\epsilon} \end{aligned}$$

Based on Kriest & Evans, Earth & Planetary Sciences, 2000



### Size spectrum comparison





# Flux Comparison



# **Biological Processes**



Stemmann et al., Deep-Sea Research I, 2004

#### **Chemical Processes**



#### Extension of Honeyman & Santschi (1989)

Burd et al., Deep-Sea Research I, 2000



# Multiple Particle Types



Burd et al., Deep-Sea Research I, 2007

Three particle types (algal cells, fecal pellets, aggregates)

Each follows a separate lognormal distribution.

Each particle type has settling velocity law, carbon content etc.

### **Multiple Particle Types**



Coagulation coupled to an ecosystem model

Jackson, Deep-Sea Research I, 2001

### Conclusions

- Need a combination of modeling approaches
  - Detailed mechanistic models & data comparisons on the same scales & same information
  - Computationally efficient models that capture the dynamics and can run in large scale models
- Need to assess the assumptions built into the models
  - How do assumptions (scientific & numerical) affect interpretation of results?
- Models & data need to inform each other