

Modeling Carbon Dynamics Using FACE Data from Duke Forest

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Luke Vaughan

Background

- Climate change in the U.S.
- CO₂ and the greenhouse effect
- C sequestration in forest ecosystems
- Duke Forest (NC)
- Loblolly pine trees (*Pinus taeda*)



Duke Forest FACE Experiment

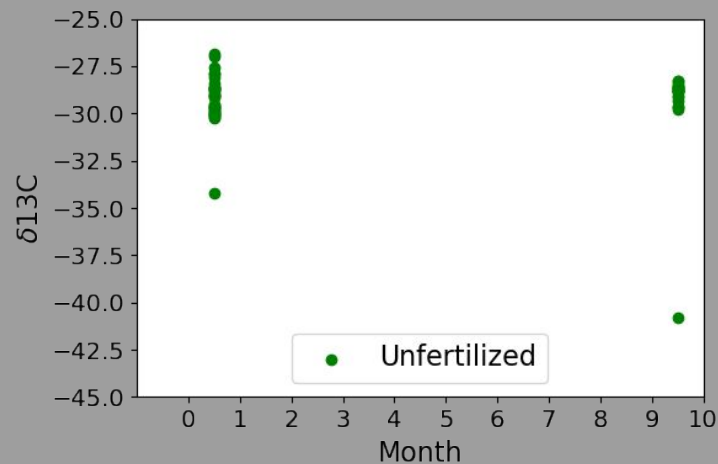
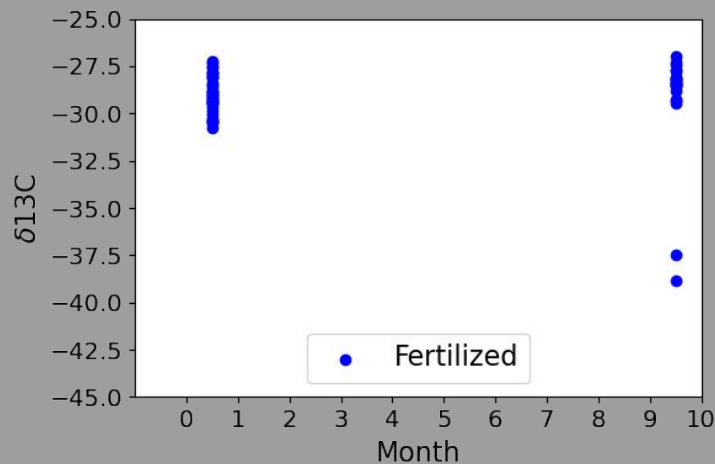
- Free-air CO₂ enrichment
- Fumigated and non-fumigated roots: $\delta^{13}\text{C}$ values



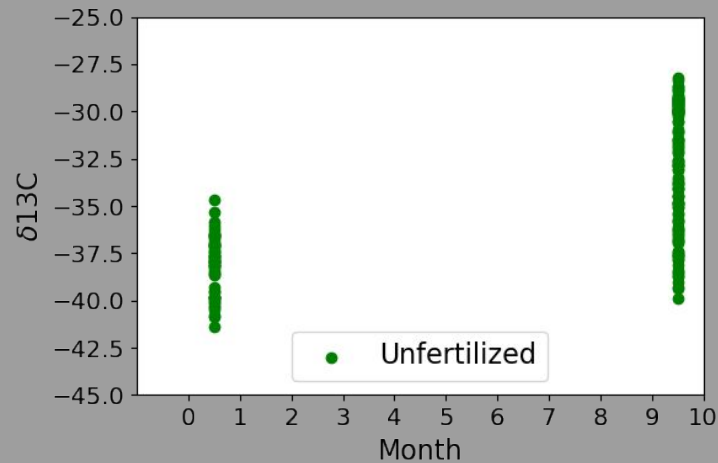
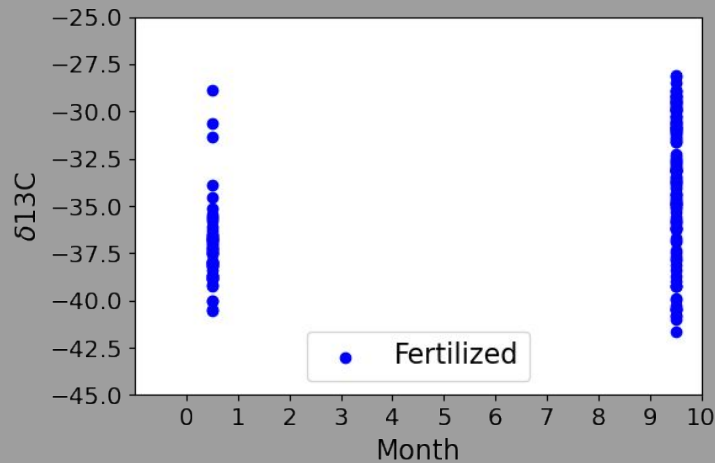
$$\delta^{13}\text{C} = \left[\frac{R(\text{sample}) - R(\text{standard})}{R(\text{standard})} \right] \times 1000\text{‰}$$
$$R = {}^{13}\text{C}/{}^{12}\text{C}$$

Data

Ambient:

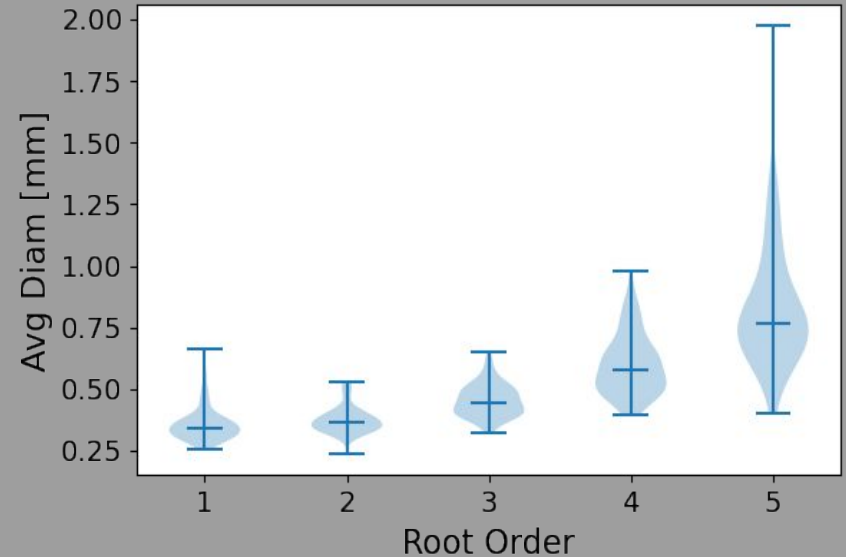
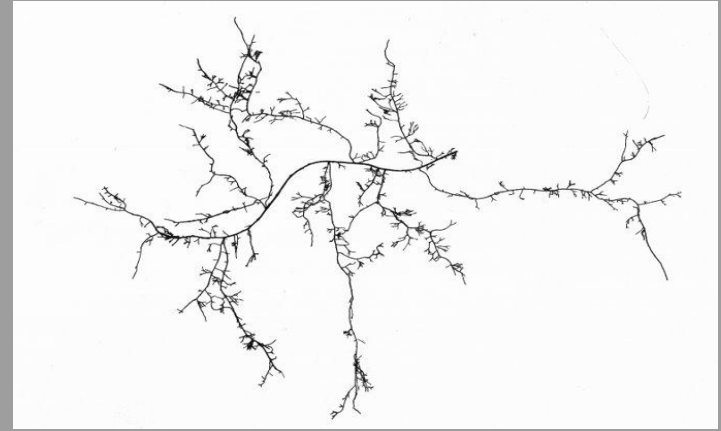
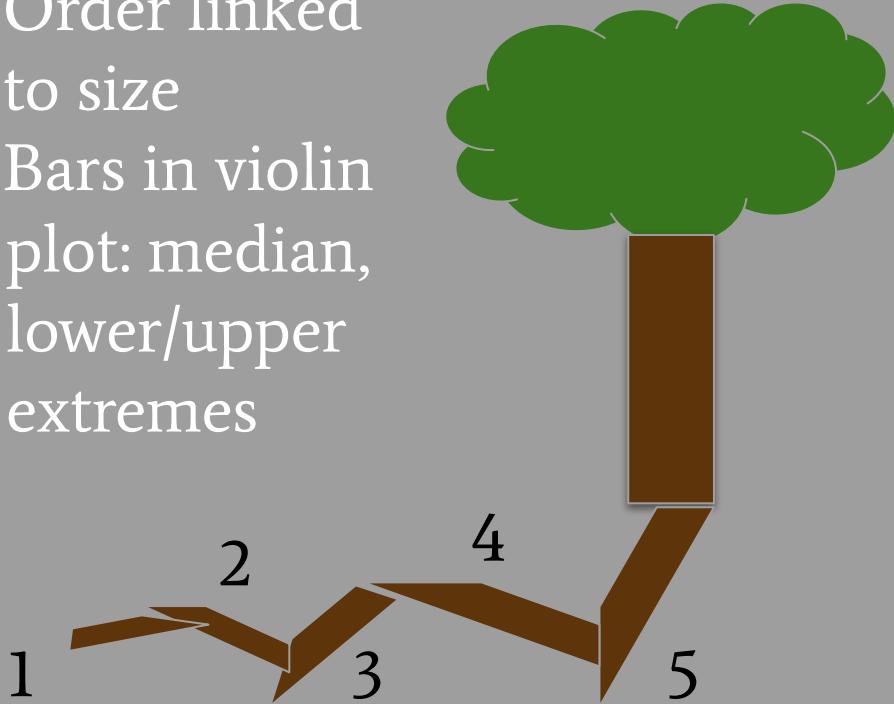


Elevated:



Root Order

- Sequential branching off
- Order linked to size
- Bars in violin plot: median, lower/upper extremes



One-Pool Carbon Model

- Linear ODE
- Solution $x(t)$ defined as $\delta^{13}\text{C}$ values at time t
- Initial condition: -42.6‰ (elevated equilibrium)
- Estimation for ambient equilibrium: -27‰
- Nonlinear regression
- One curve for each data point: extract k values

$$\frac{dx}{dt} = -k (x - x_{\text{eq}})$$

$$x(t) = Ae^{-kt} + x_{\text{eq}}$$

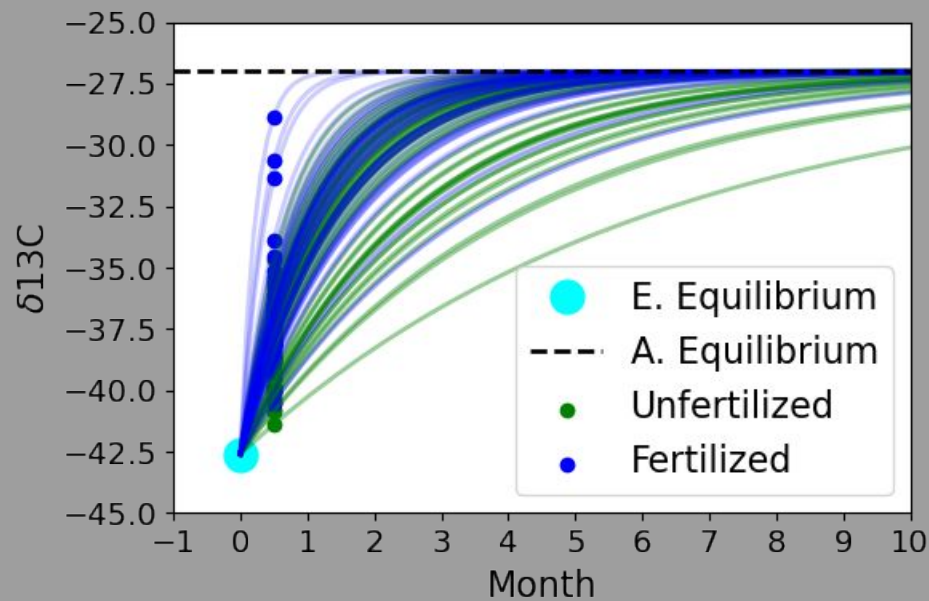
$$x(0) = -42.6$$

$$x_{\text{eq}} = -27$$

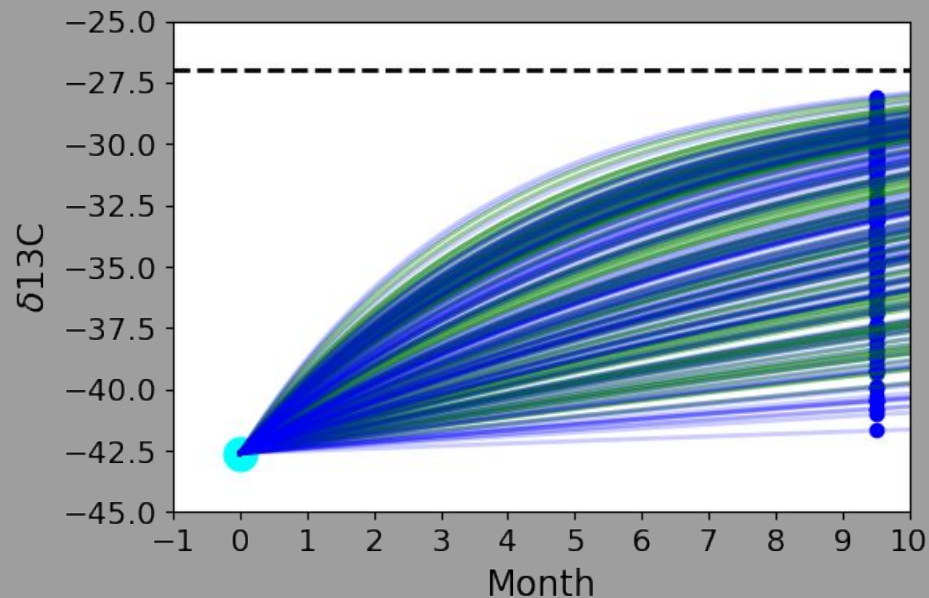
$$x(t) = -15.6e^{-kt} - 27$$

Nonlinear Regression

Short Term



Long Term

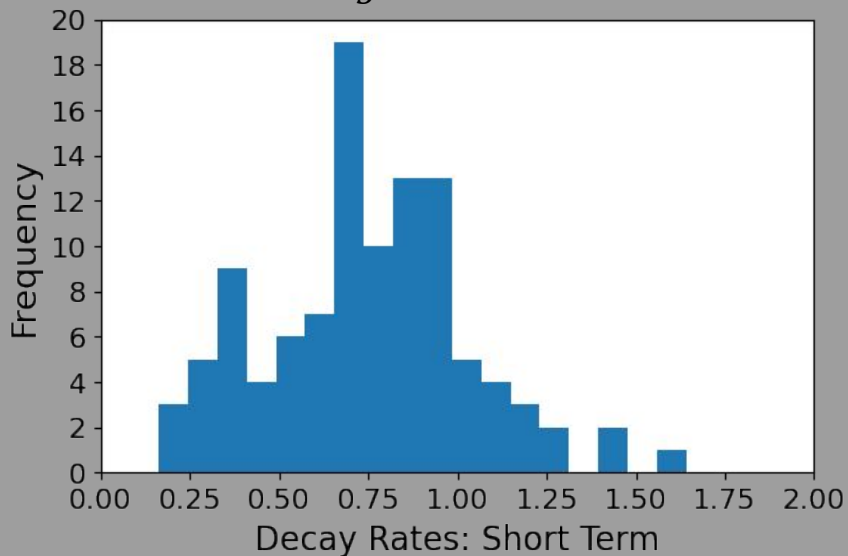


Distributions of Decay Rates by Timescale

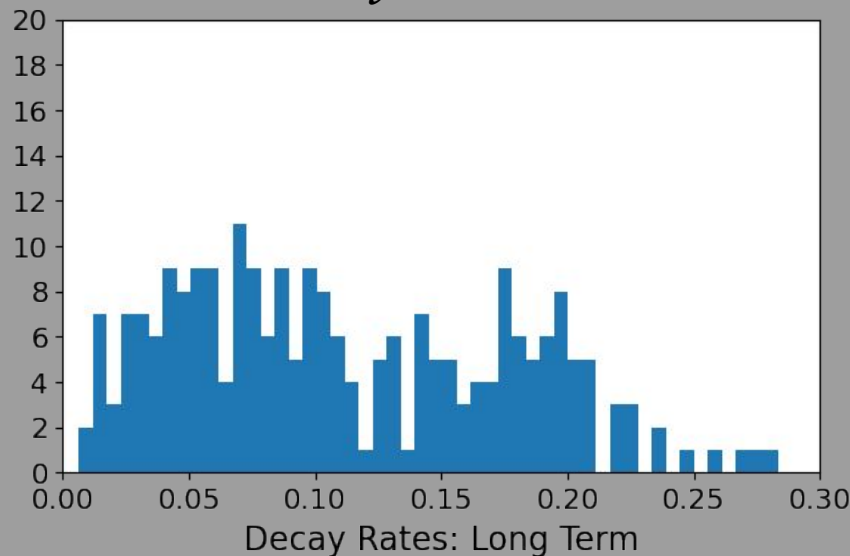
Evidence for existence of 2 timescales:

- Mean
- Range
- Distribution shape

$$\bar{k}_s = 0.82$$



$$\bar{k}_\ell = 0.11$$

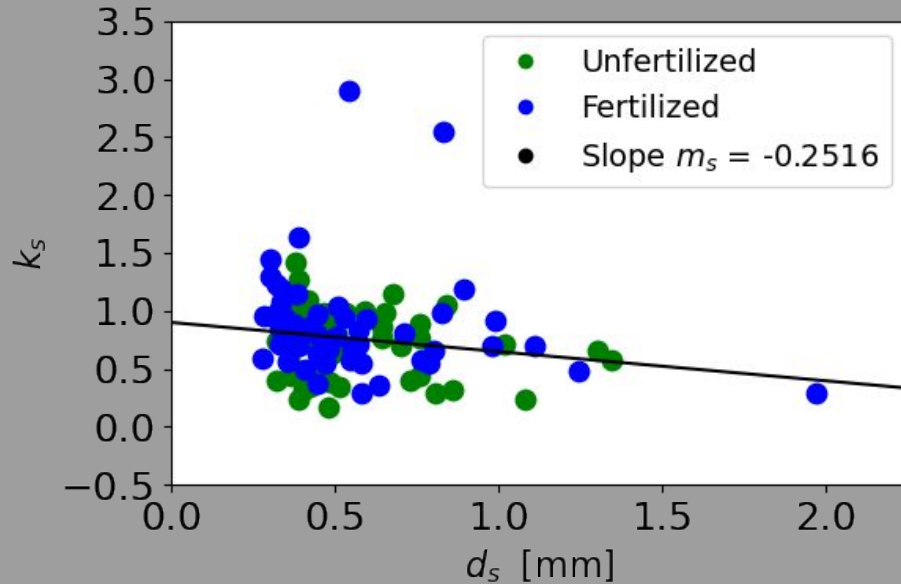


Decay Rates vs. Root Diameter

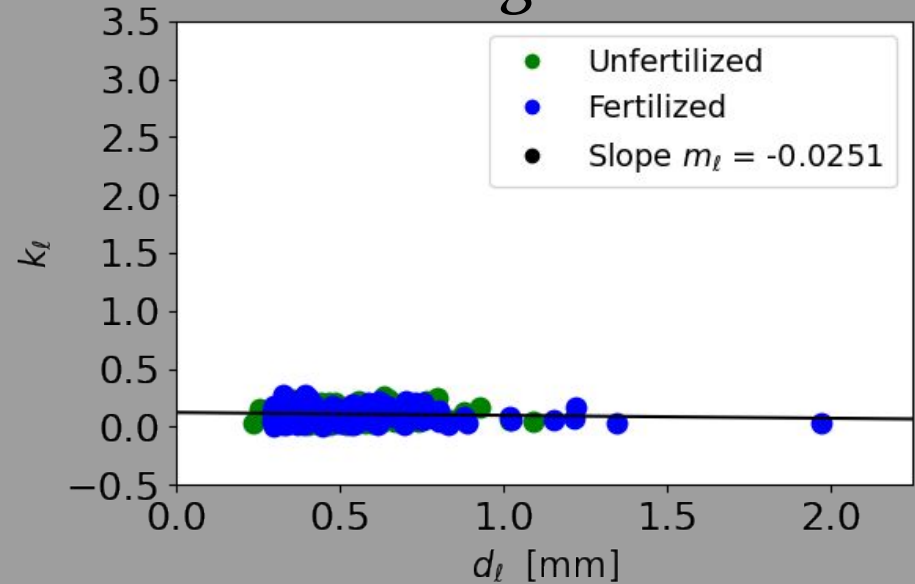
Robust linear regression:

- k_s depends on d_s
- k_ℓ does not depend on d_ℓ

Short Term

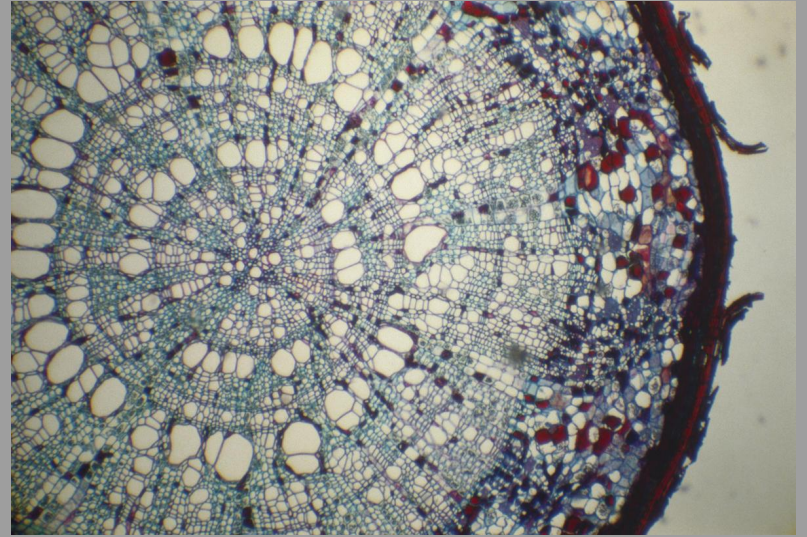


Long Term



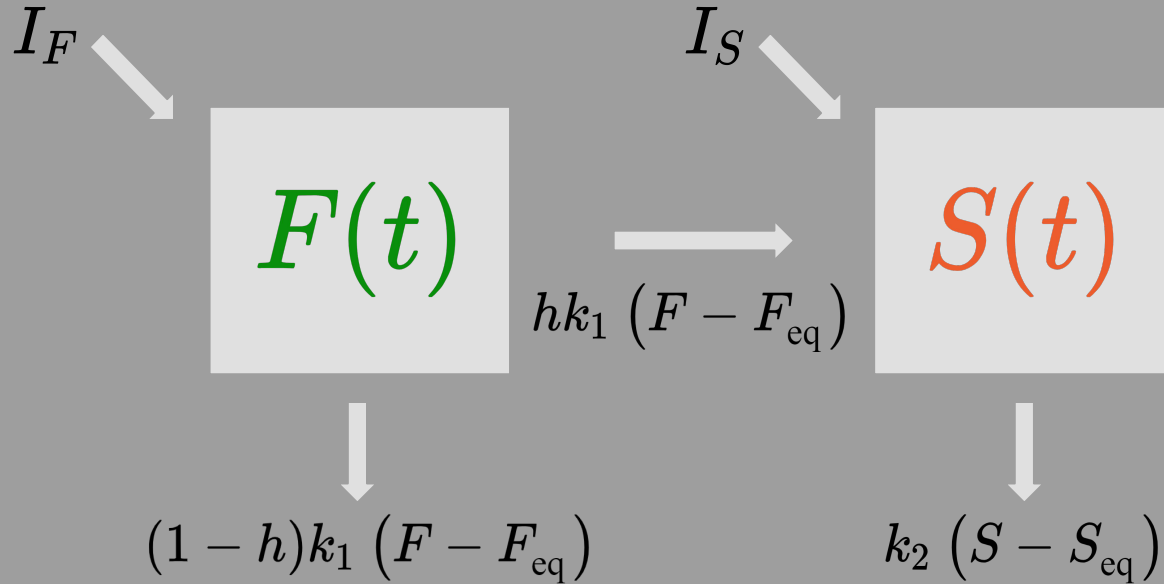
Two-Pool Carbon Model

- “Fast” & “slow” pools $F(t)$ & $S(t)$
- Respiration rates k_1 & k_2
- Equilibrium values F_{eq} & S_{eq}
- Fraction of fast converted to slow: h
- Atmospheric input I_F & I_S



Labile & recalcitrant
root material

Schematic for Two-Pool Carbon Model



$$\frac{dF}{dt} = I_F - k_1 (F - F_{eq})$$

$$\frac{dS}{dt} = I_S + hk_1 (F - F_{eq}) - k_2 (S - S_{eq})$$

Solution Derivation

- Linear ODEs
- Eigenvalue & eigenvector decomposition
- Method of undetermined coefficients
- Constraints on initial conditions & equilibrium values

$$\vec{x}' = A\vec{x} + \vec{b}$$

$$\vec{x} = \begin{bmatrix} F - F_{\text{eq}} \\ S - S_{\text{eq}} \end{bmatrix}$$

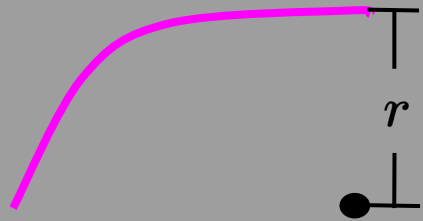
$$A = \begin{bmatrix} -k_1 & 0 \\ hk_1 & -k_2 \end{bmatrix} \quad \vec{b} = \begin{bmatrix} I_F \\ I_S \end{bmatrix}$$

$$F(0) + S(0) = -42.6$$

$$F_{\text{eq}} + S_{\text{eq}} = -27$$

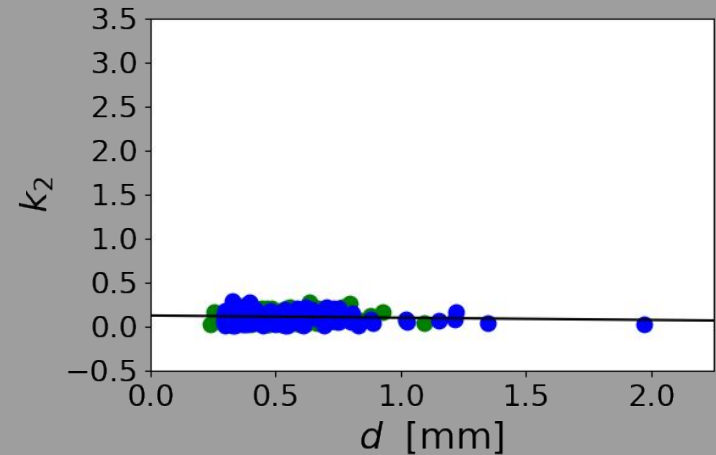
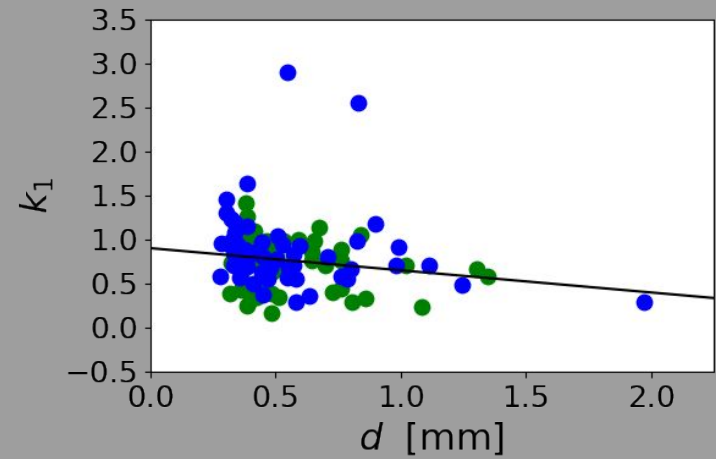
Optimization

- $T(t) = F(t) + S(t)$
- Parameters: F_0, F_{eq}, h, k_1, k_2
- Lines of best fit (robust regression):
 $k_1(d), k_2$
- SciPy's `minimize` function
- Objective function: $A(F_0, F_{eq}, h)$



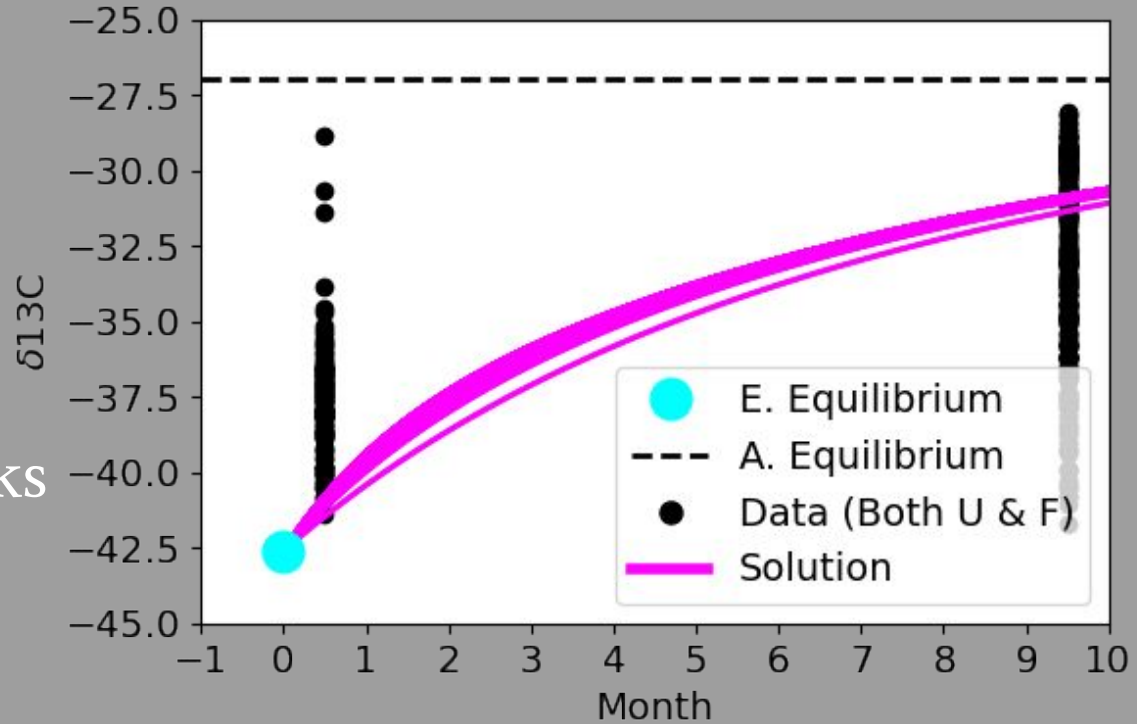
A diagram illustrating the distance r from a point to a curve. A magenta curve is shown on the left. A black dot represents a point. A vertical line segment with perpendicular end-caps connects the point to the curve, representing the distance r .

$$r = |T(t) - p|$$



Solution

- $T(t) = F(t) + S(t)$
- Minimum average residual: 3.3054
- Benefits and drawbacks of two-pool carbon model



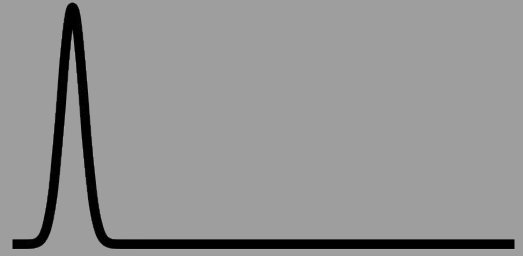
$$F(t) = -9.92e^{-k_1 t} - 10.04$$

$$S(t) = \frac{-5.65k_1}{k_2 - k_1} (e^{-k_1 t} - e^{-k_2 t}) - 5.68e^{-k_2 t} - 16.96$$

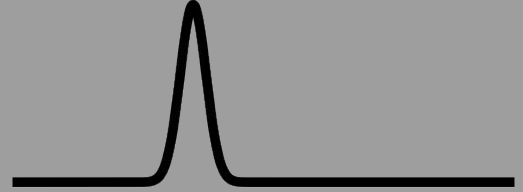
Spatial Dependence

- Spatial extension of two-pool carbon model
- Carbon as a traveling wave in one dimension
- Reaction-advection-diffusion (RAD) equations
- Root respiration, carbon transport, spread of particles

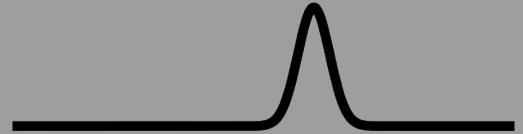
$$t = t_0$$



$$t = t_1$$



$$t = t_2$$

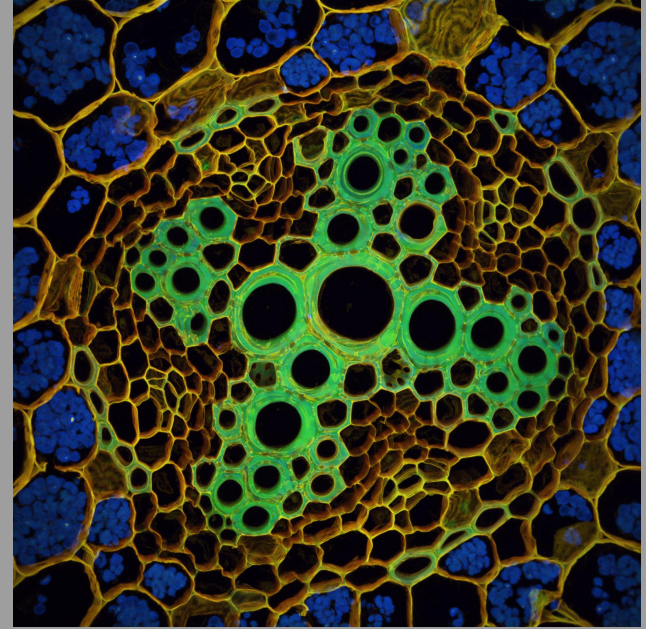


$$t = t_3$$



Qualitative PDE Model

- Fast & slow carbon concentrations C_F, C_S
- Wave speed v in fast pool only: phloem
- Diffusion coefficients D_F, D_S with $D_F \gg D_S$



$$\frac{\partial C_F}{\partial t} = -k_1 (C_F - C_{F\text{eq}}) + \frac{\partial}{\partial x} (v C_F) + \frac{\partial^2}{\partial x^2} (D_F C_F)$$
$$\frac{\partial C_S}{\partial t} = h k_1 (C_F - C_{F\text{eq}}) - k_2 (C_S - C_{S\text{eq}}) + \frac{\partial^2}{\partial x^2} (D_S C_S)$$

Model Analysis

- Two IBVPs
- Notation: $C_F = u(x,t)$, $C_S = r(x,t)$
- Wave speed $v = c$
- Map RAD equation to diffusion equation
- Explicit solution: Fourier series

Fast:

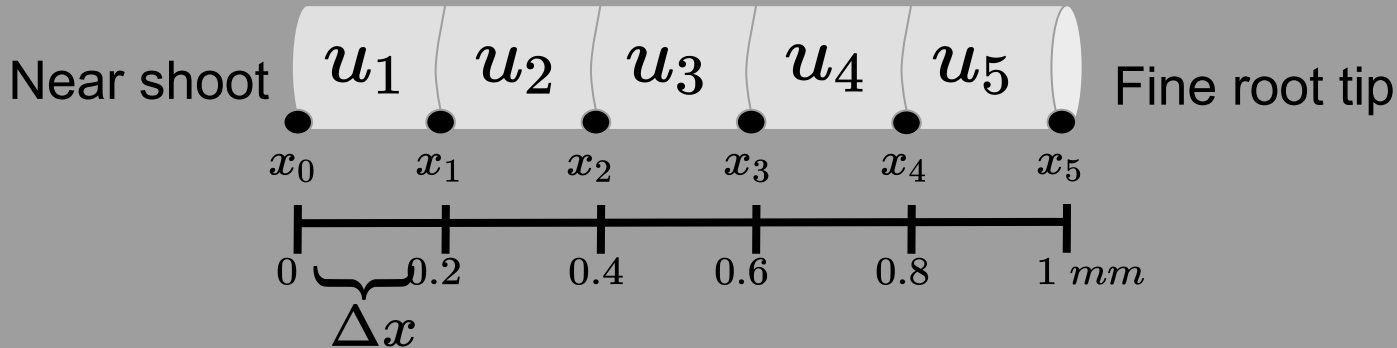
$$\begin{cases} u_t = -k_1 (u - u_{\text{eq}}) + cu_x + D_F u_{xx} \\ u(0, t) = f(t) & u(L, t) = 0 \\ u(x, 0) = g_F(x) \end{cases}$$

Slow:

$$\begin{cases} r_t = hk_1 (u - u_{\text{eq}}) - k_2 (r - r_{\text{eq}}) + D_S r_{xx} \\ r_x(0, t) = 0 & r_x(L, t) = 0 \\ r(x, 0) = g_S(x) \end{cases}$$

Numerical Simulation

- Spatial discretization: example with $N = 5$, $L = 1$ mm with $\Delta x = L/N$
- Solution at node x_i approximated as $u(i\Delta x, t) \approx U_i$ (fast) and $r(i\Delta x, t) \approx R_i$ (slow)



Finite Differences

- System of ODEs for interior nodes

$$U'_i = -k_1 (U_i - u_{\text{eq}}) + c \left[\frac{U_{i+1} - U_{i-1}}{2\Delta x} \right] + D_F \left[\frac{U_{i+1} - 2U_i + U_{i-1}}{(\Delta x)^2} \right]$$

$$R'_i = hk_1 (U_i - u_{\text{eq}}) - k_2 (R_i - r_{\text{eq}}) + D_S \left[\frac{R_{i+1} - 2R_i + R_{i-1}}{(\Delta x)^2} \right]$$

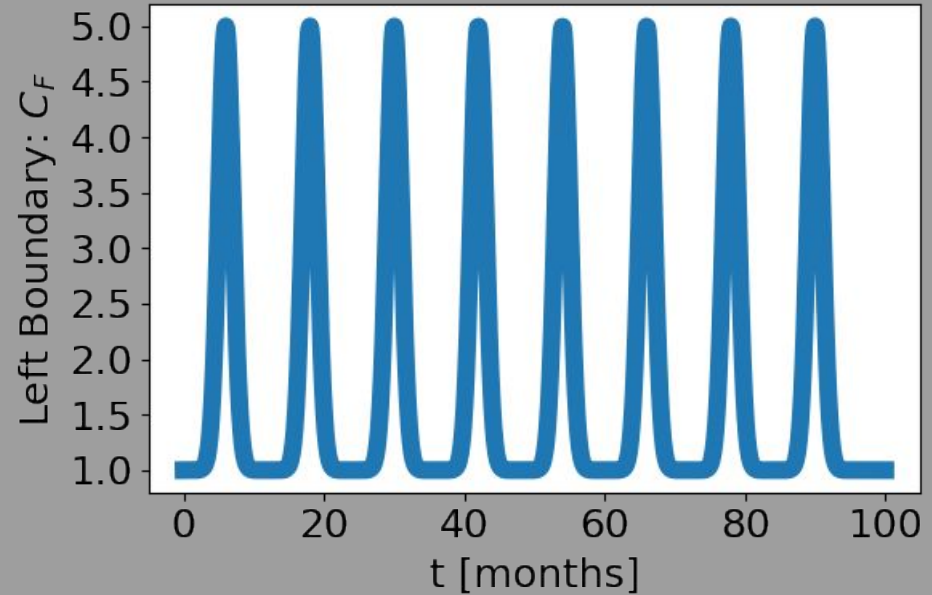
- Crank-Nicolson method: discretize time with uniform Δt

$$w_t = f(t, x, w, w_x, w_{xx})$$

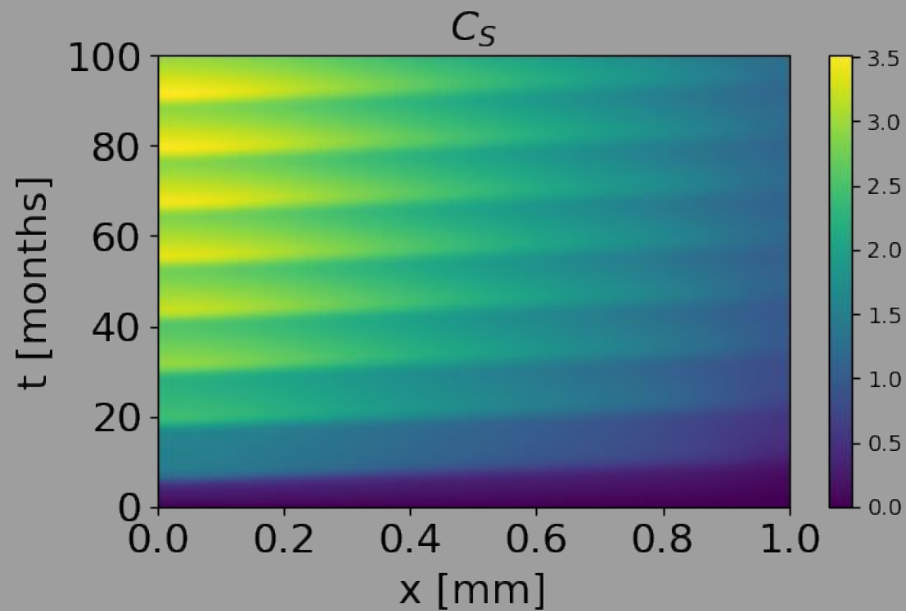
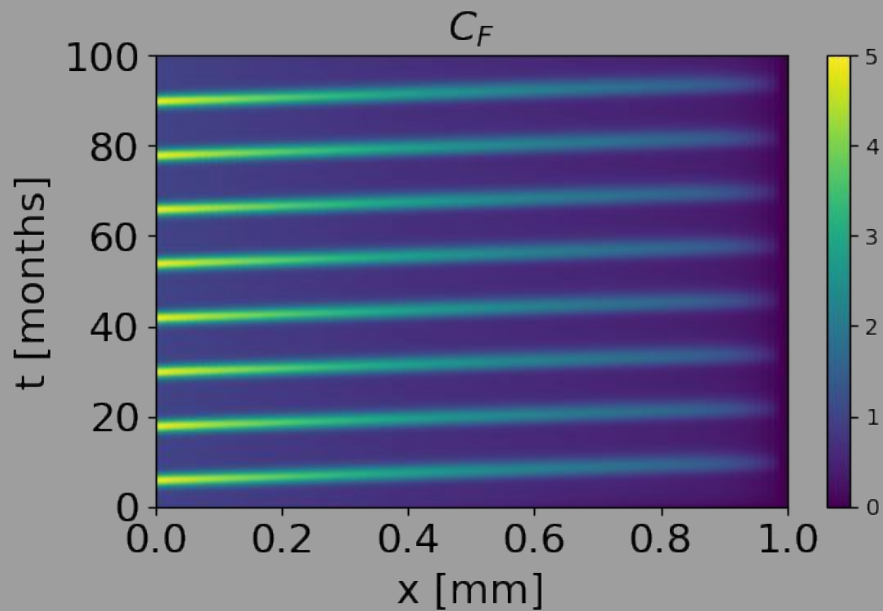
$$w_i^{k+1} = w_i^k + \frac{\Delta t}{2} [f_i^k(t, x, w, w_x, w_{xx}) + f_i^{k+1}(t, x, w, w_x, w_{xx})]$$

Simulation 1

- Left boundary condition for fast carbon: $C_F = f(t)$
- Seasonal fluctuations
- Sum of Gaussian curves
- Initial conditions: lines satisfying Dirichlet and Neumann boundary conditions

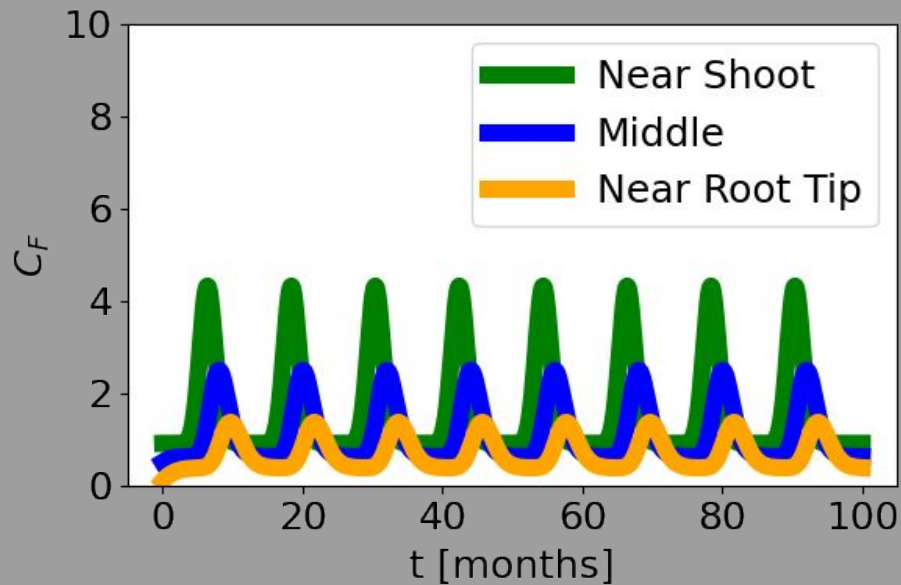


Simulation 1: Color Plots

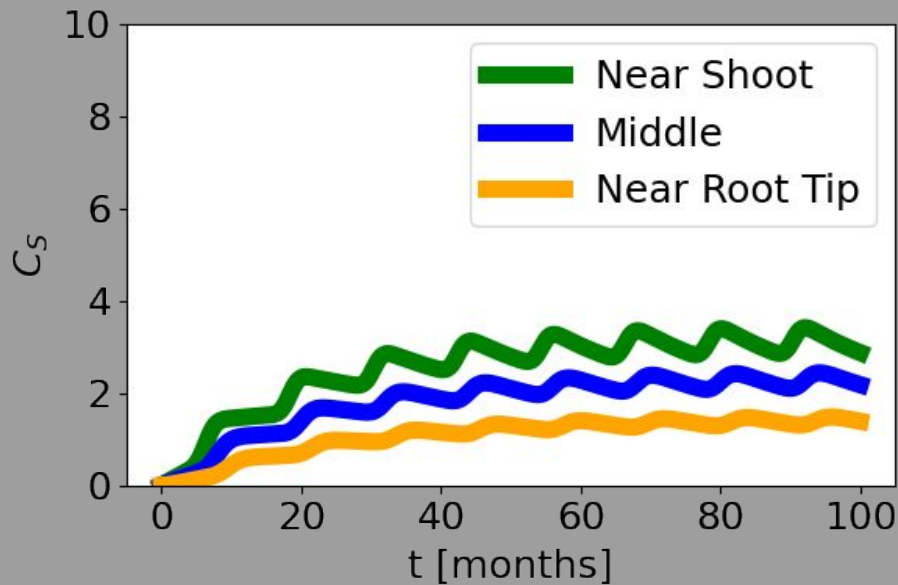


Simulation 1 (cont.)

Fast Carbon

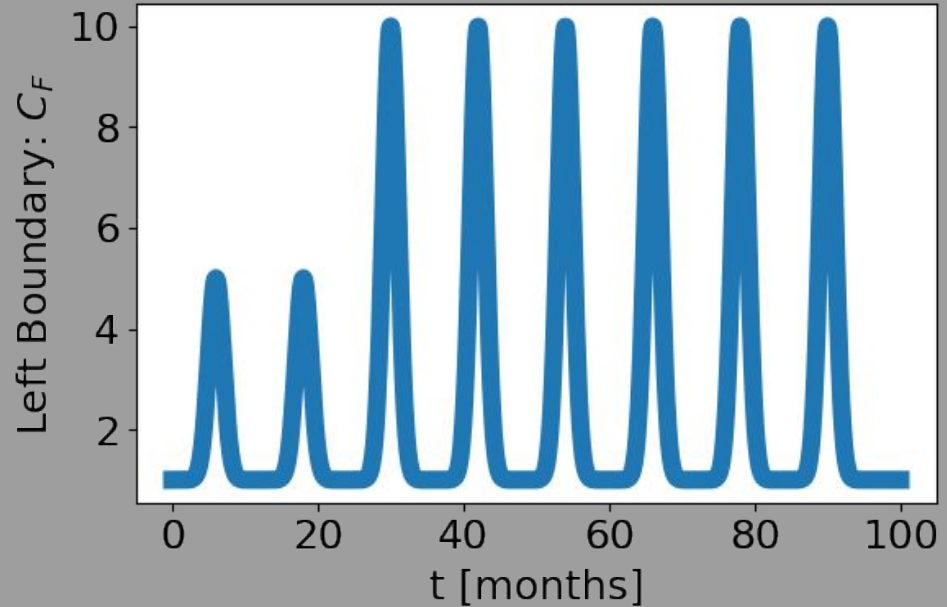


Slow Carbon

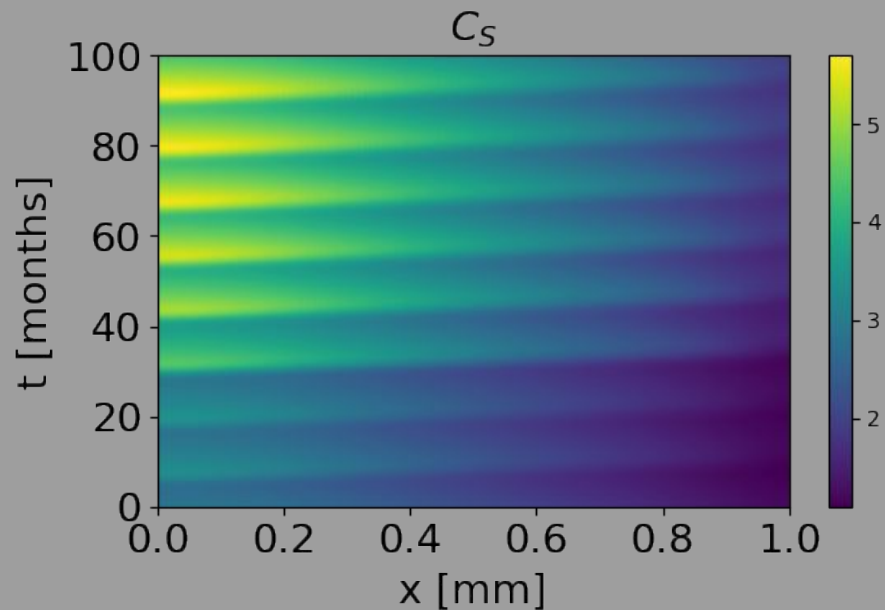
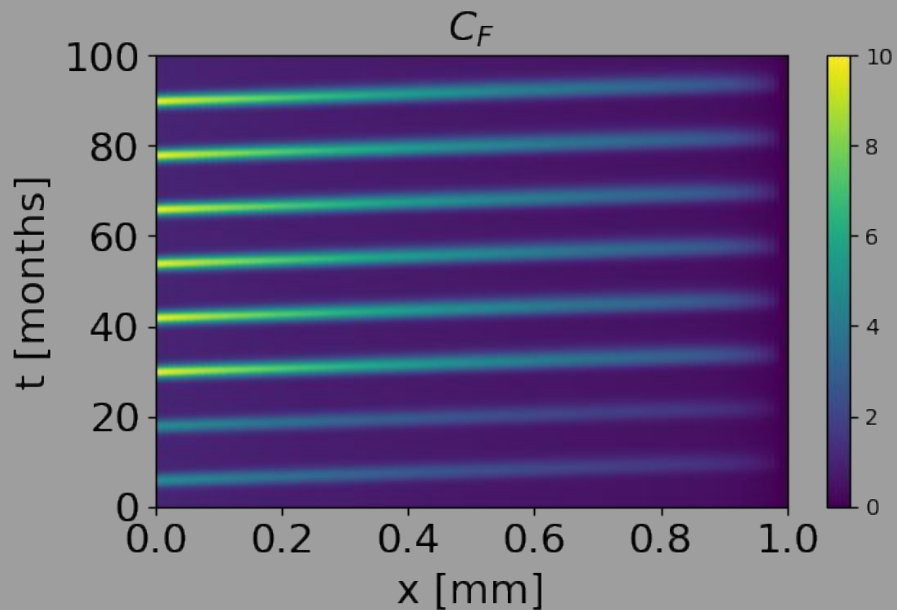


Simulation 2

- Ambient & elevated conditions
- Shift from ambient to elevated near $t = 30$
- Initial conditions: solutions from simulation 1 at steady state (last time step)

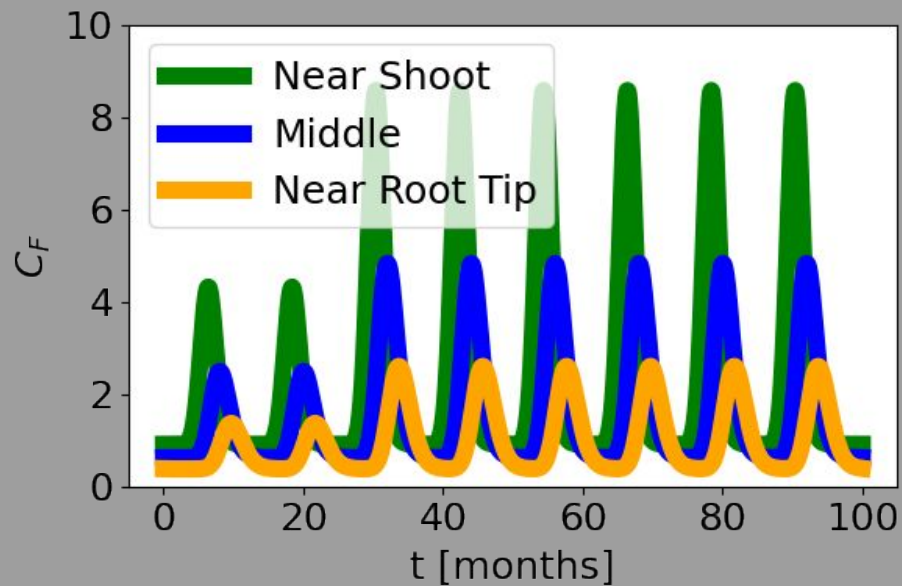


Simulation 2: Color Plots

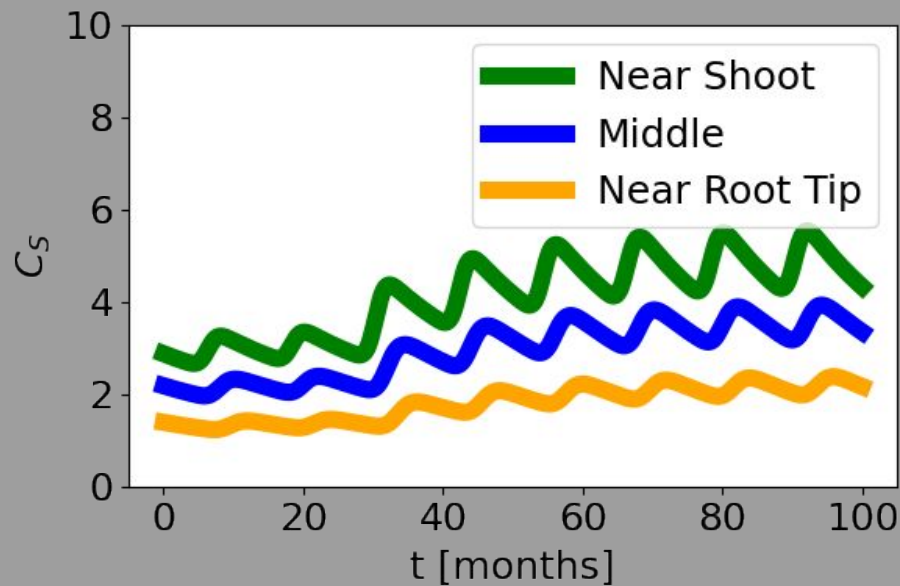


Simulation 2 (cont.)

Fast Carbon



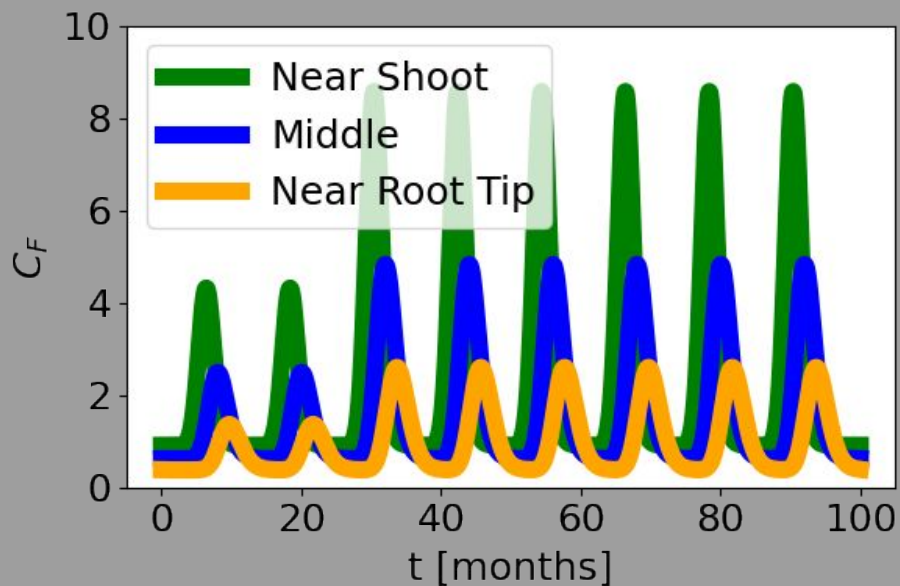
Slow Carbon



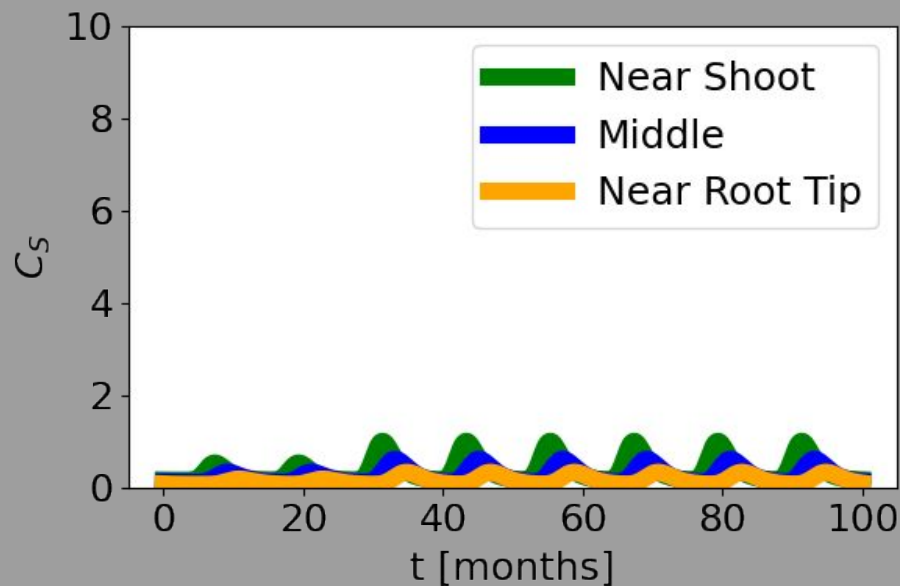
Simulation 3

$$k_2 = 0.05 \longrightarrow k_2 = 0.6$$

Fast Carbon



Slow Carbon



Conclusions

- Carbon dynamics: $\delta^{13}\text{C}$, root diameter, and root order
- C-only vs. C-N models
- One-pool model: poor fit to data
- Two-pool model: improvement with some benefits and drawbacks
- PDE model for single root
- Future directions: nonlinear respiration and extension to root network

