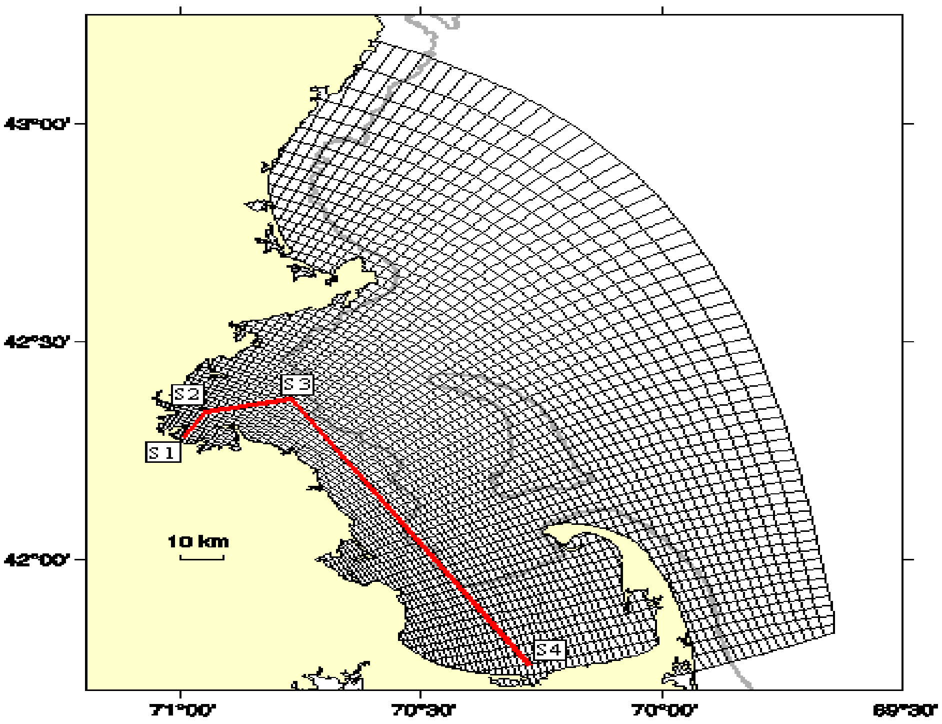
Water Quality Models: Types, Issues, Evaluation

Major Model Types

- Finite Difference
- Finite Element
- Harmonic Models
- Methods of Characteristics (Eulerian-Lagrangian Models)
- Random Walk Particle Tracking

Finite Difference



MWRA, 1996

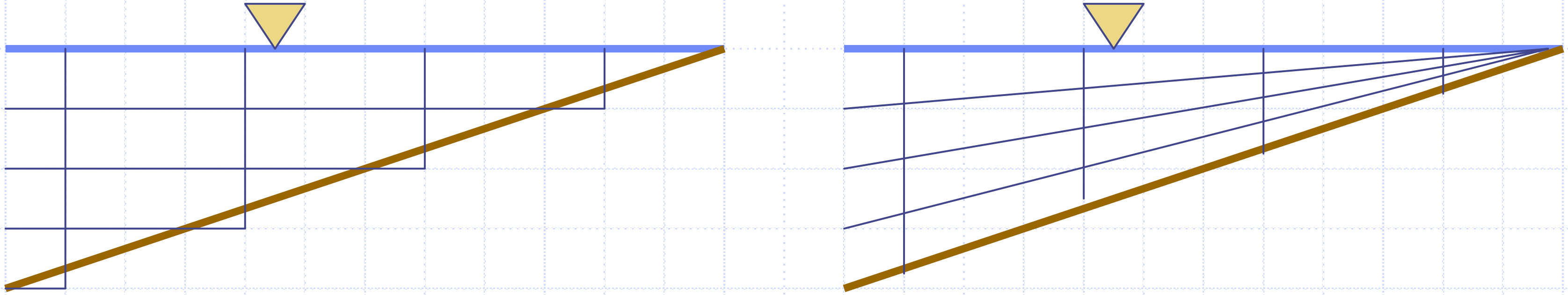
- Differential eq. => difference eqn.
- Choices of grids in horizontal and vertical (orthogonal)
- Different orders of approximation in space and time
- Large matrices, solved interatively

Example Codes

- 3-D
  - Princeton Ocean Model
  - Regional Ocean Modeling System (ROMS)
  - GLLVHT Model
  - EFDC
- 2-D depth averaged
  - WIFM-SAL
- 2-D laterally averaged
  - LARM
- 1-D Cross-sectional-averaged
  - QUAL2E
- 1-D Horizontally-averaged
  - DYRESM
  - WQRRS
  - MITEMP

Grids

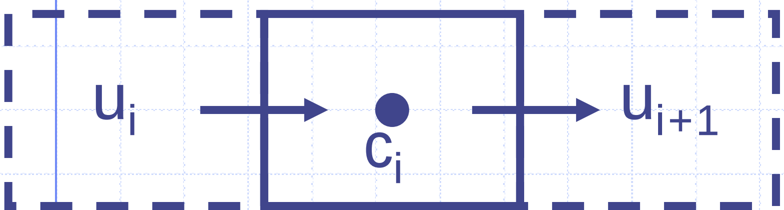
- Horizontal
  - Rectangular
  - Orthogonal
- Vertical
  - Stair-stepped (z coordinate)
  - Bottom fitting (σ coordinate)



Also isopycnal models

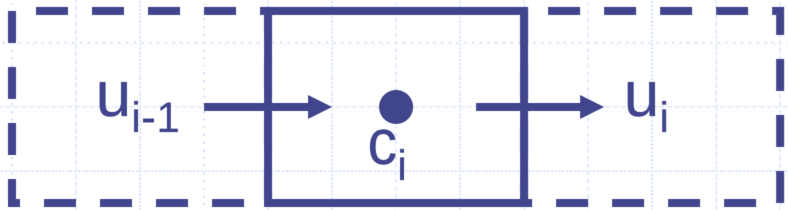
Finite Difference (1-D examples)

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} + E\frac{\partial^2 c}{\partial x^2}$$



Cell "i"

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}(uc) + E\frac{\partial^2 c}{\partial x^2}$$



Cell "i"

$$\frac{c_i^{\,n+1} - c_i^{\,n}}{\Delta t} = -\frac{u_i(c_i - c_{i-1})}{\Delta x} + E\left(\frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2}\right) \qquad \text{A}$$

$$= -\left(\frac{u_i c_i - u_{i-1} c_{i-1}}{\Delta x}\right) + E\left(\frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2}\right) \qquad \text{B}$$

B from conservative (control volume) form of eqn

Time stepping

- Explicit (evaluate RHS at time n)

A $$c_i^{n+1} = c_i^{n}[1 - \frac{u_i \Delta t}{\Delta x} - \frac{2E\Delta t}{\Delta x^2}] + c_{i-1}^{n}[\frac{u_i \Delta t}{\Delta x} + \frac{E\Delta t}{\Delta x^2}] + c_{i+1}^{n}[\frac{E\Delta t}{\Delta x^2}]$$

- Implicit (evaluate RHS at time n+1)

A $$[-\frac{u_i \Delta t}{\Delta x} - \frac{E\Delta t}{\Delta x^2}]c_{i-1}^{n+1} + [1 + \frac{u_i \Delta t}{\Delta x} + \frac{2E\Delta t}{\Delta x^2}]c_i^{n+1} - \frac{E\Delta t}{\Delta x^2}c_{i+1}^{n+1} = c_i^n$$

Solution involves tri-diagonal matrix

Time stepping (cont'd)

- Mixed schemes
  - e.g., Crank-Nicholson wts n, n+1 50% each
- Numerical accuracy and stability depend on

$$\frac{u\Delta t}{\Delta x}$$ Courant Number

$$\frac{E\Delta t}{\Delta x^2}$$ Diffusion Number

being less than critical values (~1)

Finite Element

- Information stored at element nodes
- Approx sol'n to differential eqn.
- Large matrices, solved iteratively
- More flexible than FD
- Somewhat more overhead

Example Codes

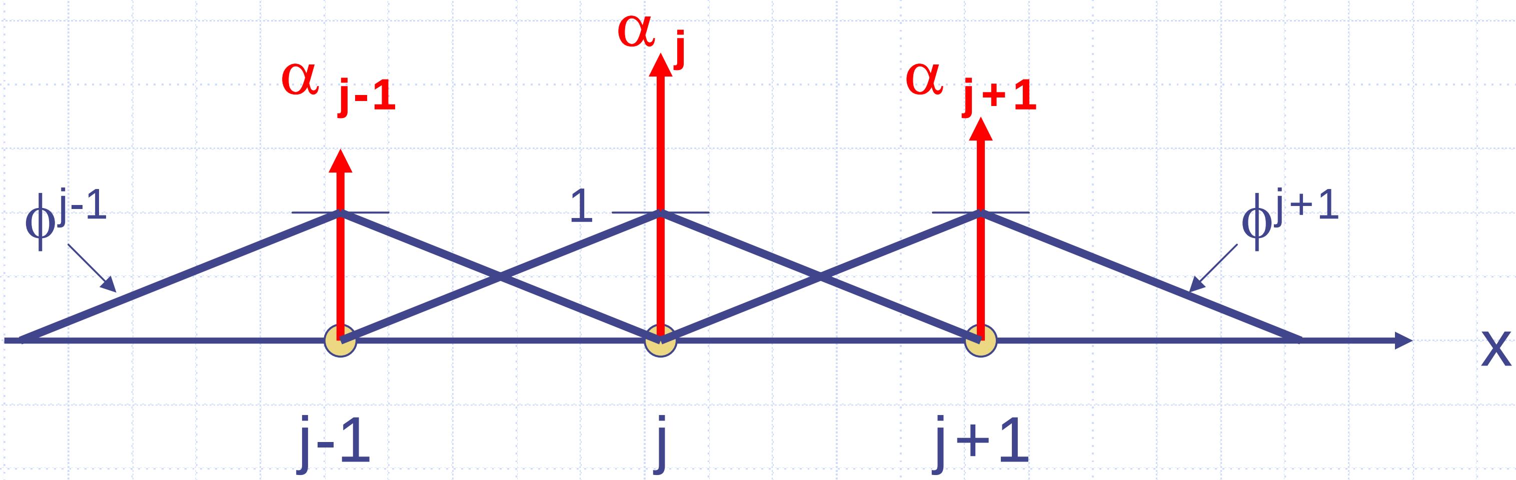
- 3-D
  - RMA-10 and –11
- 2-D Horizontal Average
  - EDF
  - ADCIRC
  - RMA-2 and -4

Finite Element (1-D example)

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - E\frac{\partial^2 c}{\partial x^2} = 0$$

$$c(x,t) \cong \hat{c}(x,t) = \sum_{j=1}^{N_T} \alpha_j(t)\phi^j(x)$$

real c discrete c unknowns interpolationg fns



Finite Element (1-D example)

R = residual = discrete equation – real equation

$$= \frac{\partial \hat{c}}{\partial t} + u \frac{\partial \hat{c}}{\partial x} - E \frac{\partial^2 \hat{c}}{\partial x^2}$$

W = weighted residual

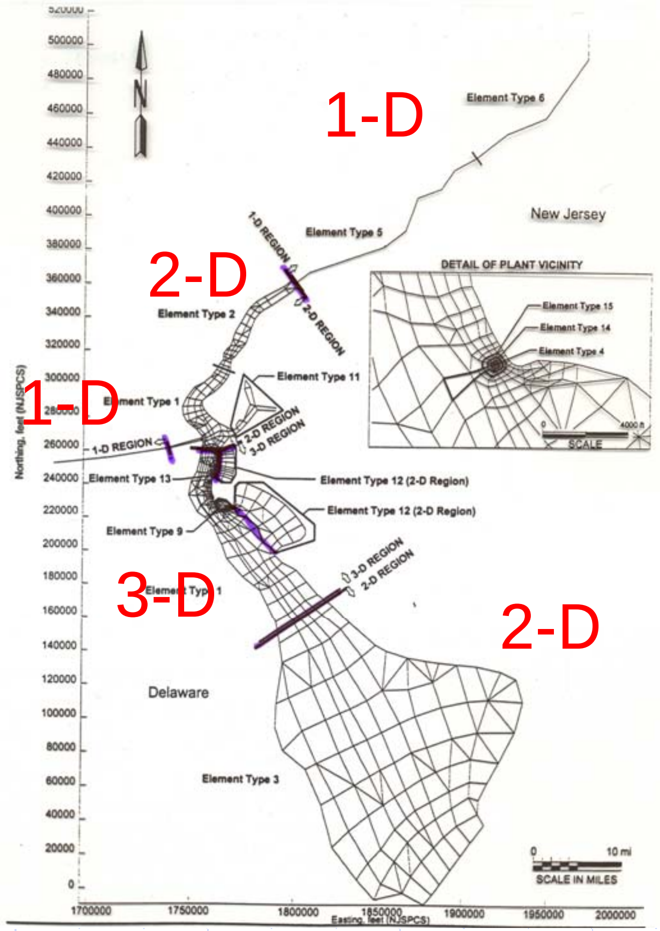
$$= \int_0^L wRdx = 0$$

weighting functions ϕ^j

Account for boundary conditions as well

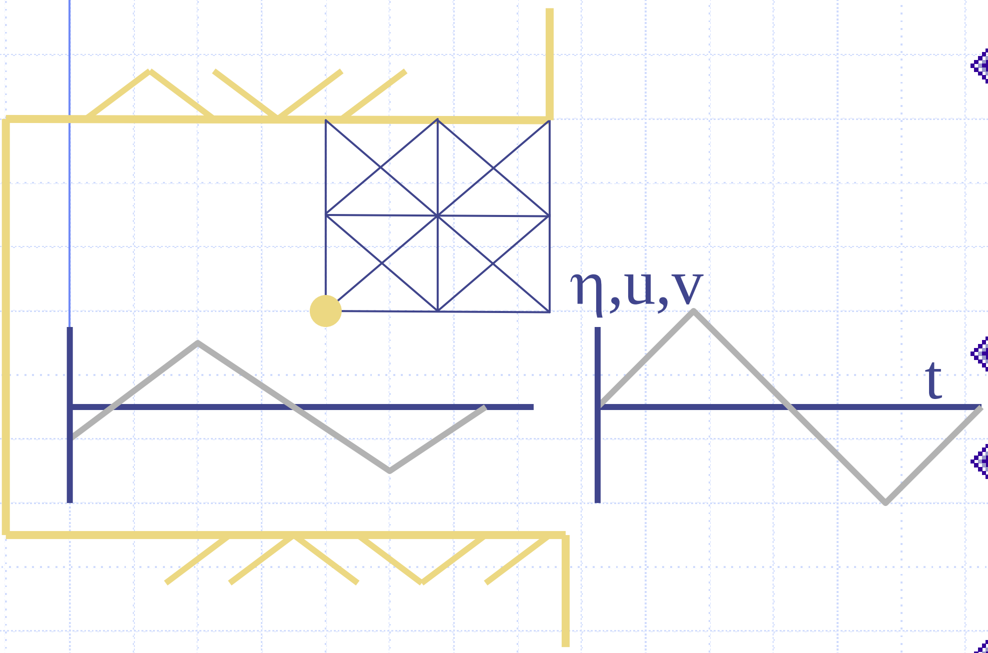
Different element dimensions

- Finite element grid (RMA10/11) for Delaware R
- 1-D, 2-D and 3-D elements



PSEG, 2000

Harmonic Models



- Periodic motion outside => periodic motion inside
- Plus harmonics
- Transient problem => steady problem
- Best for tidally-dominated flows

Example Codes

- 3-D
  - Lynch et al. (Dartmouth)
- 2-D Horizontal
  - Tidal Embayment Analysis (MIT)

Harmonic Decomposition

$$\eta(x,y,t) = A_\eta(x,y)\cos(\omega t + \phi_\eta) = A_\eta^* e^{i\omega t}$$

$$u(x,y,t) = A_x^* e^{i\omega t}$$

$$v(x,y,t) = A_y^* e^{i\omega t}$$

Ex.

$$\frac{\partial \eta}{\partial t} = A_\eta^* (i\omega) e^{i\omega t}$$

$$h\frac{\partial u}{\partial x} = h\frac{\partial A_x^*}{\partial x} e^{i\omega t}$$

$$h\frac{\partial v}{\partial y} = h\frac{\partial A_y^*}{\partial y} e^{i\omega t}$$

$$i\omega A_n^* \cancel{e^{i\omega t}} + h\frac{\partial A_x^*}{\partial x}\cancel{e^{i\omega t}} + h\frac{\partial A_y^*}{\partial y}\cancel{e^{i\omega t}} = 0$$

TEA-Basic Equations

$$\frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x}(uh) + \frac{\partial}{\partial y}(vh) = -\frac{\partial}{\partial x}(u\eta) - \frac{\partial}{\partial y}(v\eta)$$

$$\frac{\partial u}{\partial t} + g\frac{\partial \eta}{\partial x} - fv + \frac{\lambda u}{h} - \frac{\tau_x^s}{\rho h} = -u\frac{\partial u}{\partial x} - v\frac{\partial u}{\partial y} - \frac{\tau_{x,nl}^b}{\rho h}$$

$$\frac{\partial v}{\partial t} + g\frac{\partial \eta}{\partial y} + fu + \frac{\lambda v}{h} - \frac{\tau_y^s}{\rho h} = -u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} - \frac{\tau_{y,n\ell}^b}{\rho h}$$

Linear Terms Non-Linear Terms

Westerink et al. (1985)

Non-linear Terms

- Products of sine/cosine functions produce new sine/cosine functions with sums and differences of frequencies

Ex:

$$\cos\alpha\cos\beta = \frac{1}{2}\cos(\alpha-\beta) + \frac{1}{2}\cos(\alpha+\beta)$$

$$if \quad \alpha = \beta = \omega t = \frac{2\pi t}{T}$$

$$\cos^2(\omega t) = \frac{1}{2} + \frac{1}{2}\cos(2\omega t)$$

M_2 tide
(T = 12.4 hr)

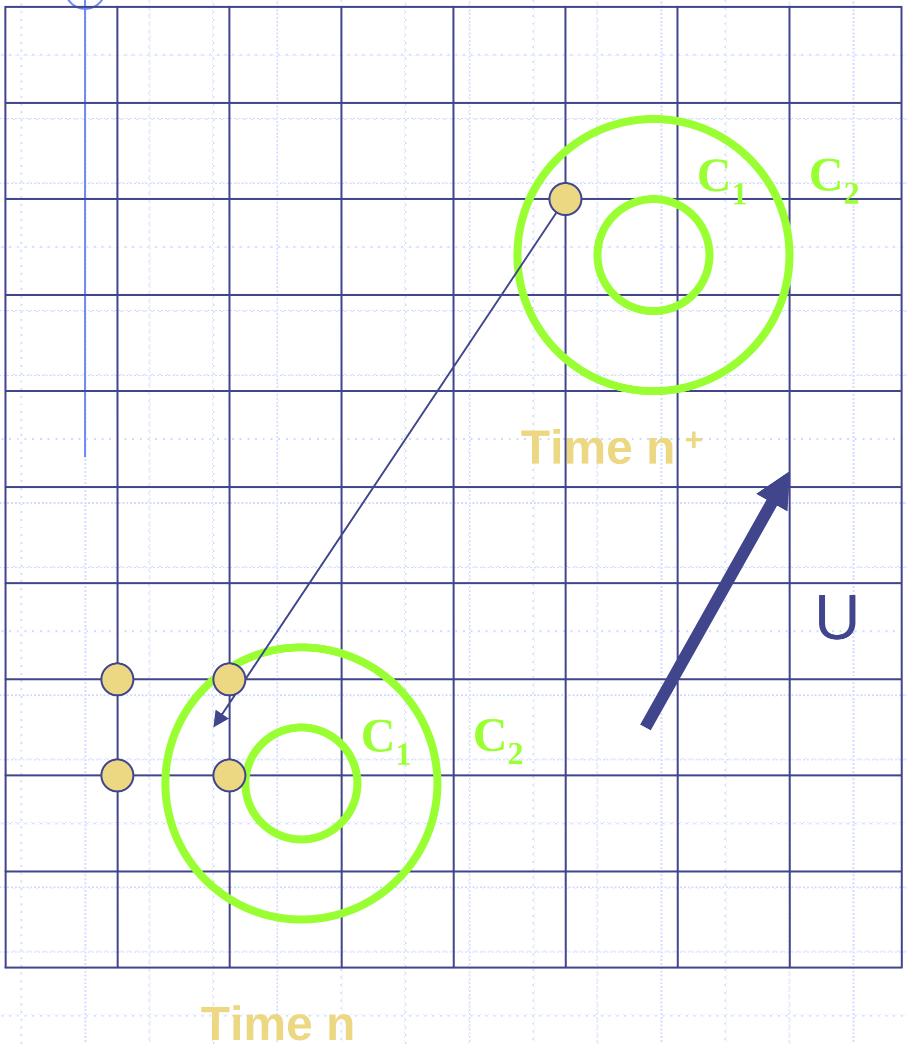
M_4 tide
(T/2 = 6.2 hr)

Non-linear forcing terms determined by iteration.

Eulerian-Lagrangian Analysis (ELA)

- Baptista (1984, 1987)
- Uses “quadratic” triangles
- Split-operator approach
  - Method of characteristics (advection)
  - FEM (diffusion/reaction)
- Puff routine
- Ideal with periodic HM input

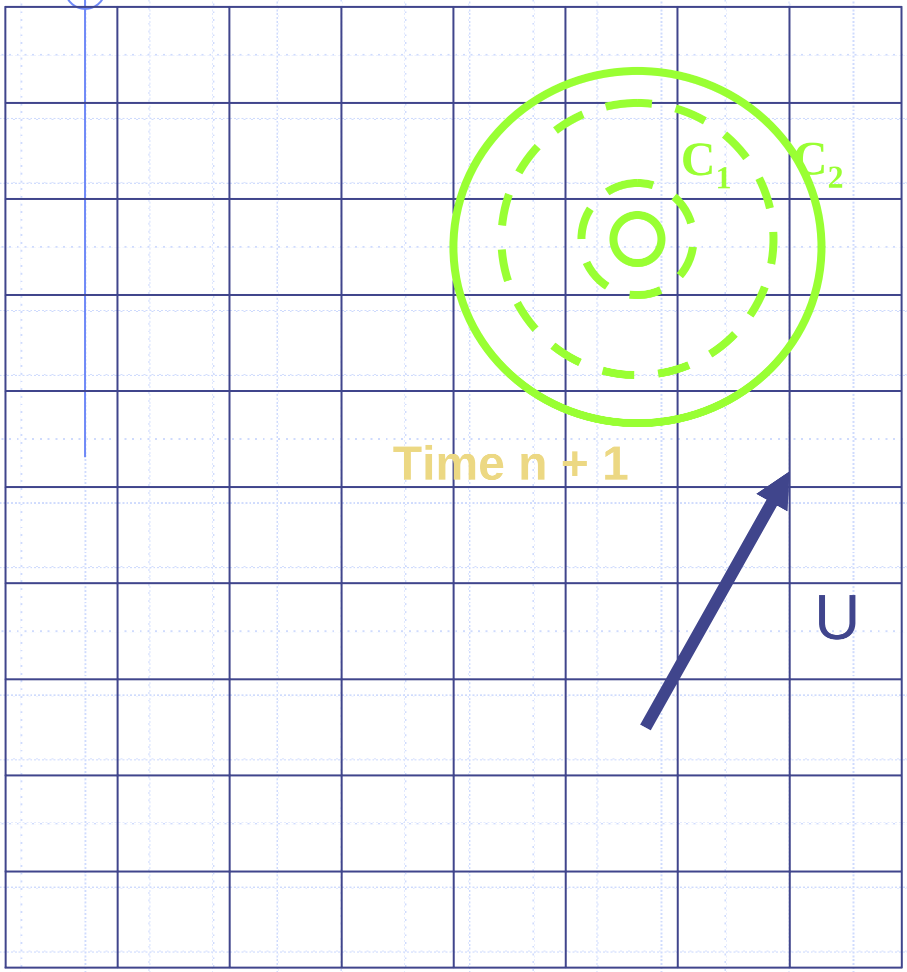
Method of Characteristics



- Backward tracking of characteristic lines
- Interpolation among nodes at feet of characteristics
- Avoids difficulties with advection-dominated flows

Baptista et al. (1984)

Diffusion



- Diffusion/simple reaction uses implicit Galerkin FEM under stationary conditions
- No stability limit on Δt
- Not intrinsically mass conserving
- Linearity facilitates source/receptor calculations

Baptista et al. (1984)

ELA-Basic Equation

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = \frac{1}{h} \frac{\partial}{\partial x_i} \left(hD_{ij} \frac{\partial c}{\partial x_j} \right) + Q$$

advection dispersion reaction

$$\frac{\partial c}{\partial t} + u_i^* \frac{\partial c}{\partial xi} = D_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j} + Q$$

$$u_i^* = u_i - \frac{1}{h} \frac{\partial}{\partial x_j} \left(hD_{ij} \right)$$

Baptista et al. (1984)

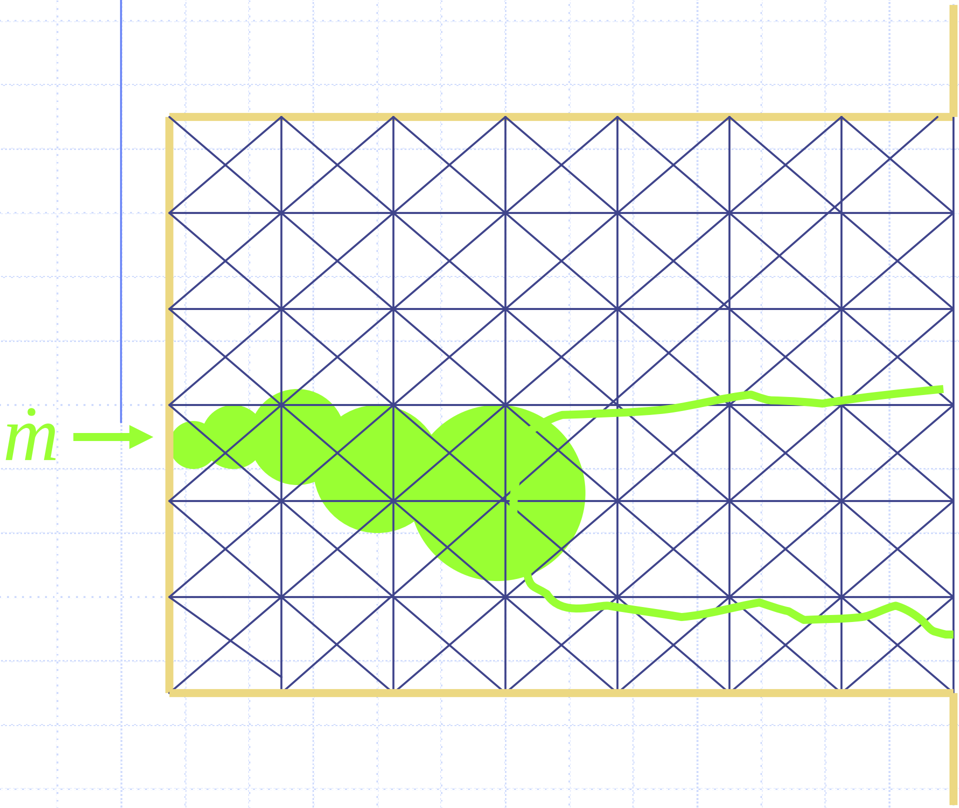
Operator Splitting

$$\frac{\partial c}{\partial t} + u_i^* \frac{\partial c}{\partial x_i} = D_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j} + Q$$

$$\frac{c^{n^+} - c^n}{\Delta t} + \left\{ u_i^* \frac{\partial c}{\partial x_i} \right\}_n = 0$$

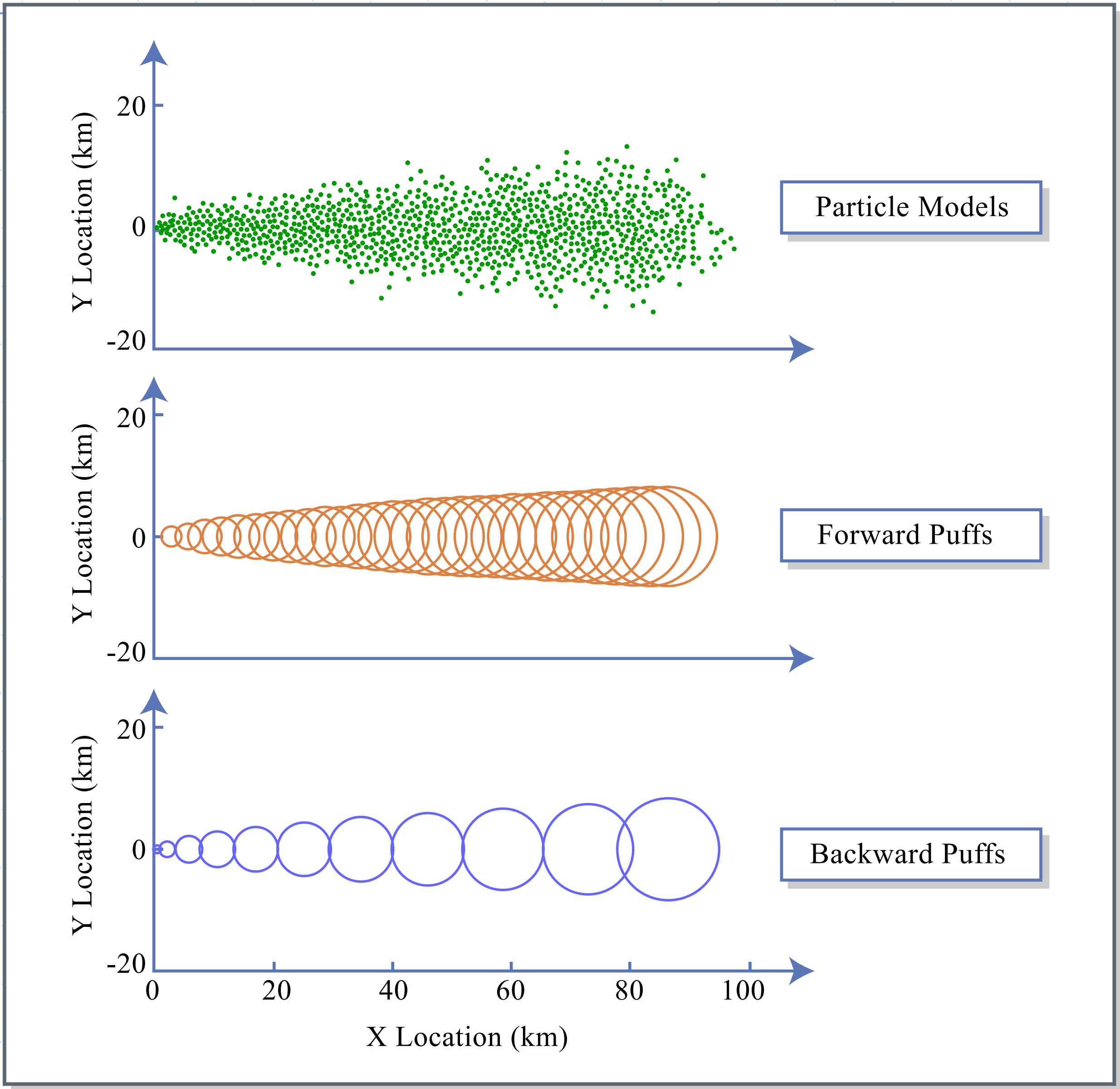
$$\frac{c^{n+1} - c^{n^+}}{\Delta t} = \left\{ D_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j} \right\}_{n+1} + \{Q\}_{n+1}$$

Puff Algorithm



- Gaussian puffs distributed backwards in time over near field
- Advected/diffused over intermediate field
- Projected to grid after sufficient diffusion (hybrid model)
- Or, self-contained model (Transient Plume Model)

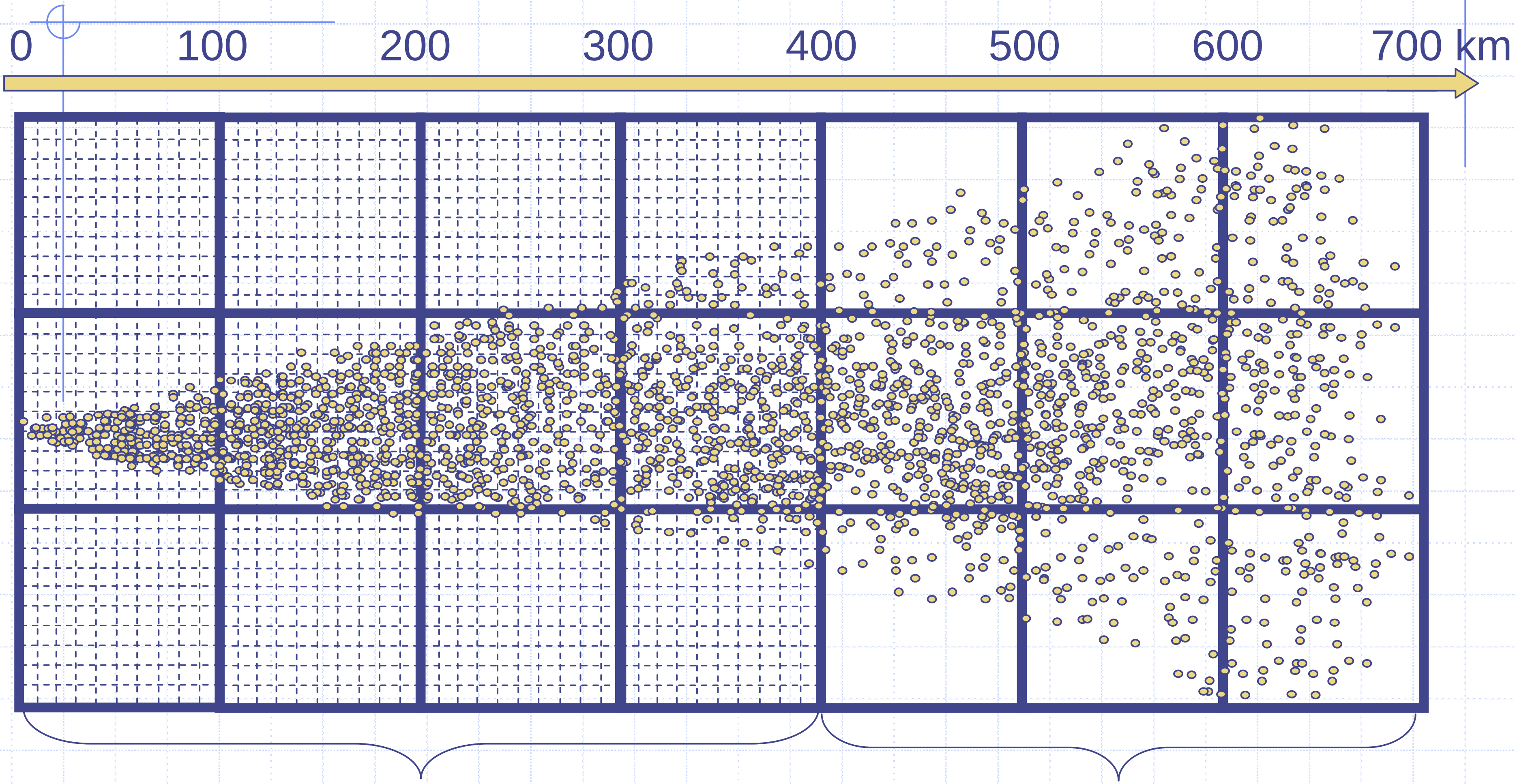
Lagrangian Models



Israelsson et al. (2006)

Figure by MIT OCW.

Hybrid Random Walk Particle Tracking/Grid Based Model



Use finer grid to visualize intermediate-field concentrations

Project particles onto OGCM grid → far-field concentrations

Application to Larval Entrainment at Coastal Power Plants

- Millstone Station on Long Island Sound
- Winter flounder larvae entrained at station intakes
- How many, what age, what proportion of local & LIS populations?

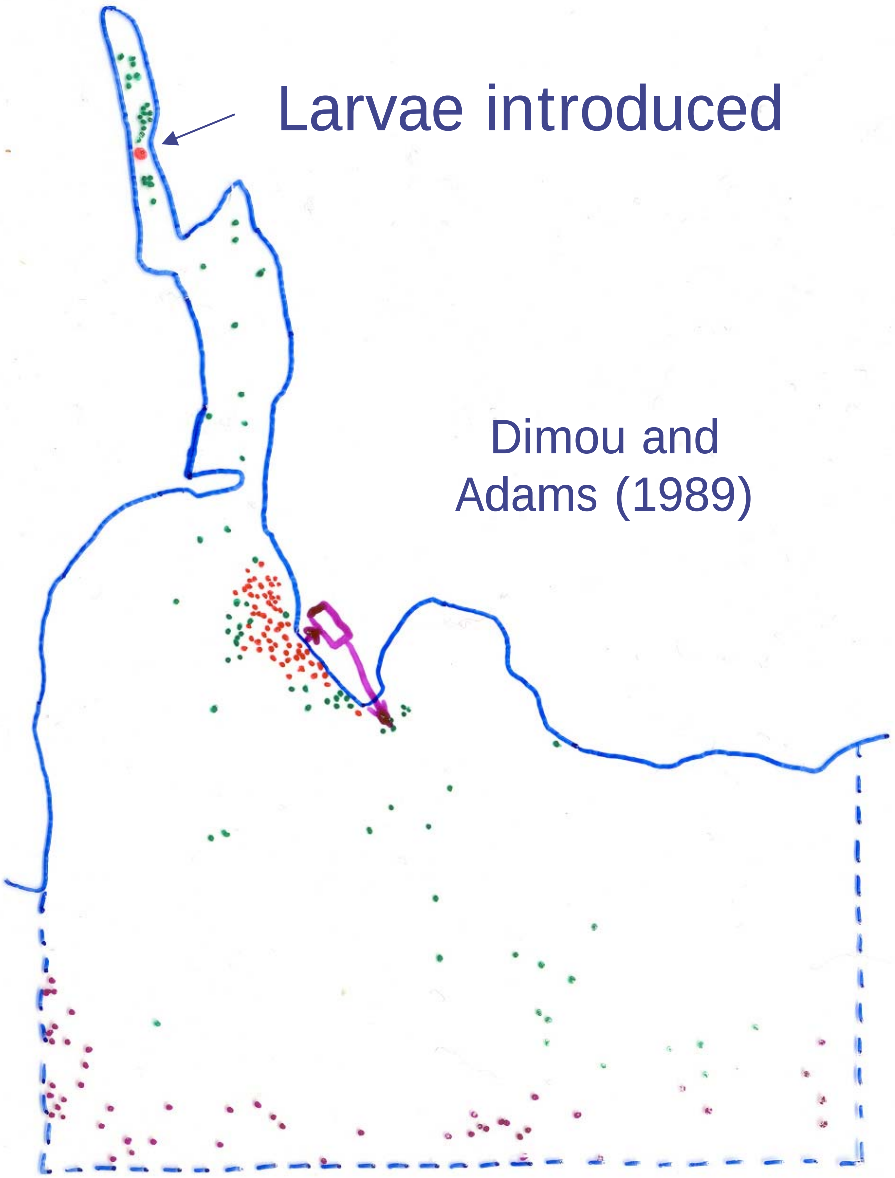
2-D Simulations

$$\Delta x_i = \left[u + \frac{\partial E_x}{\partial x} + \frac{E_x \partial h}{h \partial x} \right] \Delta t$$
$$+ \sqrt{2 E_x \Delta t}\, p_i + S / S$$

$$\Delta y_i = \left[v + \frac{\partial E_y}{\partial y} + \frac{E_y \partial h}{h \partial y} \right] \Delta t$$
$$+ \sqrt{2 E_y \Delta t}\, p_i + S / S$$

Each larva may:

- die or mature
- be entrained
- be flushed



Dye study calibration

- Dye released at Niantic River mouth
- ~20% recovered at station intake
- Accounting for mortality ~17% of larvae exiting Niantic R are being entrained

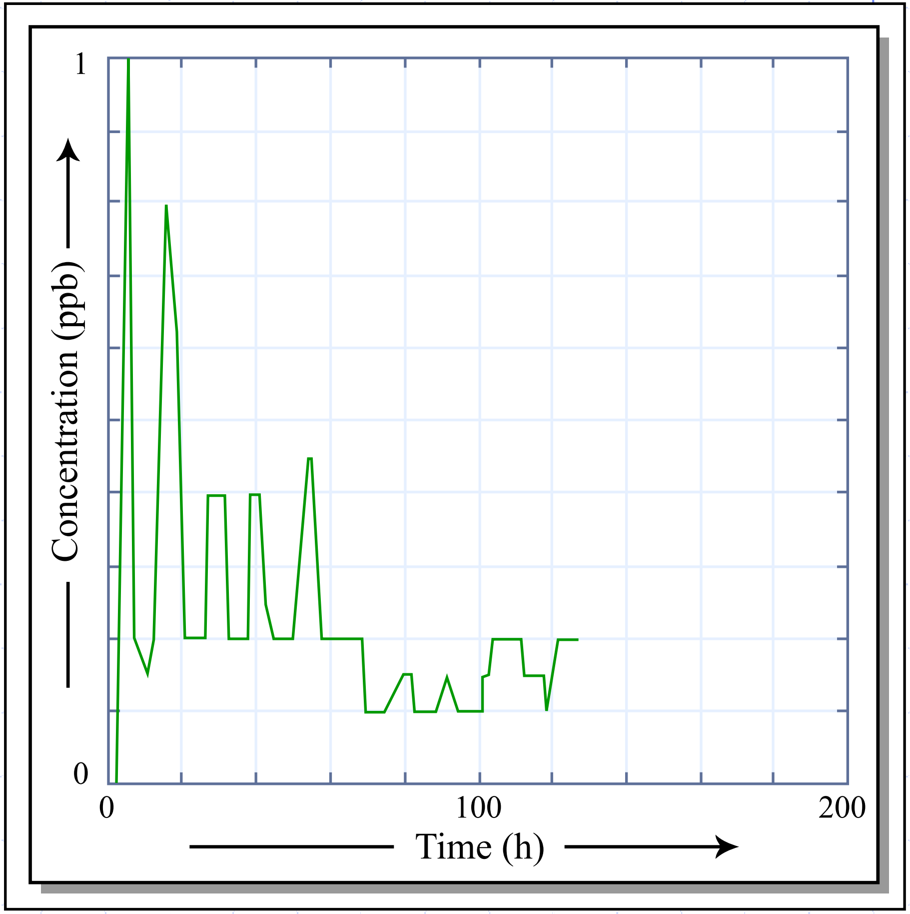
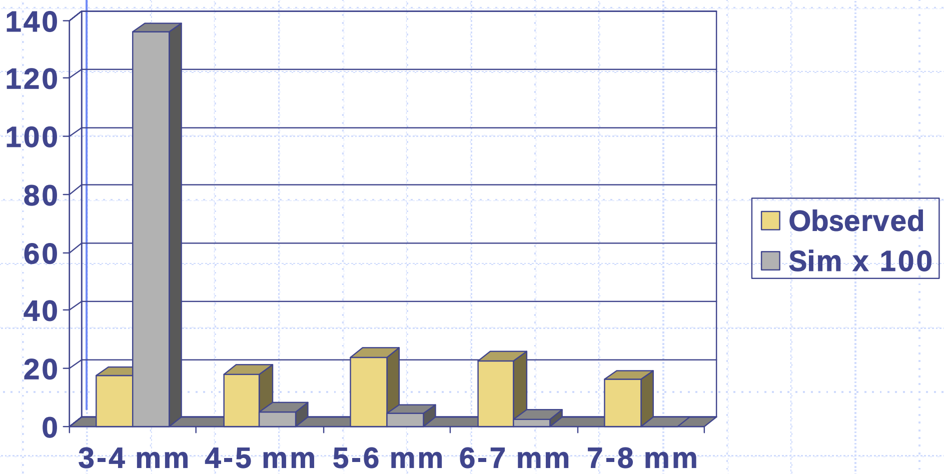


Figure by MIT OCW.

Dimou and Adams (1989)

Entrained larval lengths (10^6): observed Vs simulated



- Conclusion: most larvae imported (Connecticut and Thames Rivers)
- Supported by studies using Mitochondrial DNA and trace metal accumulation

Dimou et al. (1990)

Contemporary Issues in Surface Water Quality Modeling

- Open boundary conditions
- Inverse modeling
- Data assimilation: integrating data and model output
- Problems of spatial scale: interfacing near and far field models
- Problems of time scale: coupling hydrodynamic and water quality models

Model Performance Evaluation

aka verification, validation, confirmation, quantitative skill assessment, etc.

- Dee, D.P., "A pragmatic approach to model validation", in *Quantitative Skills Assessment for Coastal Models* (D.R. Lynch and A. M. Davies, ed), AGU, 1-13, 1995.
- Ditmars, J.D., Adams, E.E., Bedford, K.W., Ford, D.E., "Performance Evaluation of Surface Water Transport and Dispersion Models", *J. Hydraulic Engrg,* 113*:* 961-980, 1987.
- Oreskes, N., Shrader-Frechette, K., Belitz, K, Verification, Validation and Confirmation of Numerical Models in the Earth Sciences", *Science*, 263: 641-646, 1994.
- GESAMP (IMO/FAO/UNESCO/WMO/WHO/IAEA/UN/UNEP Joint Group of Experts on the Scientific Aspects of Marine Pollution), "Coastal Modeling", *GESAMP Reports and Studies, No 43*, International Atomic Energy Agency, Vienna, 1991.

Who is evaluating?

- Model Developer
  - Evaluates whether simulated processes matches real world behavior
- Model User
  - Output-oriented
  - Ability to accurately simulate conditions at specific location(s) under variety of extreme and design conditions
- Decision makers
  - Reliability, cost-effectiveness

Model Performance Evaluation*

- Problem Identification
- Relationship of model to problem
- Solution scheme examination
- Model response studies
- Model calibration
- Model validation

*Ditmars, *et al*., 1987,

Model Performance Evaluation*

- Natural System
- Conceptual Model
- Algorithmic Implementation
- Software Implementation

*Dee, 1995

Problem Identification

- What are the important processes and what are their space and time scales?
- Ex: If biogeochemical transformations are quicker than the hydraulic residence time, then perhaps steady state is OK

Relationship of model to problem

- Does model do what you concluded was important?
- Direct simulation or parameterization?
- Are data adequate to resolve the processes, initial conditions and boundary conditions?

Solution scheme examination

- Is scheme consistent with differential equations?
- Are mass, vorticity, etc. preserved?
- Choice of grid scheme, time and space steps as they affect stability and accuracy.
- Is model well documented?

Model response studies

- Does model behave as expected for simple cases?
- Does model match analytical solutions (some call this and previous step verification, connoting truth)
- Provides sensitivity to be used in model calibration.

Model calibration

- Best model fit against a known data set.
- Make sure output is appropriate
  - tidal currents vs amplitude
  - residual vs instantaneous currents
- Only tweak appropriate input parameters/coefficients.
  - physically relevant
  - those requiring least change relative to expected range of variation.

Model validation

- Comparison against independent data set (or a different period of time) without changing model parameters/coefficients.
- Choice of appropriate metrics (mean error, rms error, etc).
- Perfect agreement not possible; but are results believable? (Validity connotes legitimacy)
- Oreskes et al. (1994) refers to model confirmation

Additional Comments

- Absolute vs Relative accuracy
  - Latter is easier as uncertainties may cancel when comparing options under same conditions
- Uncertainty (as measured by output variation) during sensitivity tests)
  - Usually underestimated because of unknown unknowns
- Generic versus site-specific models
  - Will model be used at different site?

Additional Comments

- Purpose of models is insight
  - they book keep what we already think we know