

## **Modeling Myths**

- Modeling is Difficult
- Numerical models can do everything
- Numerical models will solve your problems

## **Modeling Facts**

- Modeling is simple book-keeping (plus a bit of magic)
- There are no black boxes!
- Numerical models have a life of their own and make their own problems

Used carefully, numerical solutions are a very powerful tool for gaining insight into possible physical processes. Used indiscriminately, they become an intellectual black-hole. We need to emphasize the two end-member approaches to modeling

1. **The Kitchen Sink Approach:** Throw everything into it and hope something useful comes out (BAD IDEA)
2. **The Model Problem Approach:** Gain insight by developing simple model problems that balance interesting behaviour with comprehensibility (GOOD IDEA – but takes finesse).

This course will stress the 2nd approach and will emphasize the following axioms

- Be problem driven
- Understand your problem
- Keep it simple
- Never model more than you can understand (or observe?)
- Avoid the 'reality trap' (models  $\neq$  'reality')
- Choose your techniques to mimic the underlying physics.
- The only successful model is an insightful model.

Or more succinctly

- **Think** before you model
- **Think** while you model
- **Think** after you model

## **Some Earth science problems you ought to know (maybe)**

1. Thermal convection (2-D Rayleigh-Benard)
2. The Lorenz Equations ( Chaos and ODE's)
3. The shallow water equations
4. Seismic wave propagation
5. Flow in Porous Media

## Thermal Convection (2-D Rayleigh Benard Convection)

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \nabla^2 T$$

$$\frac{1}{\text{Pr}} \left[ \frac{\partial \omega}{\partial t} + \mathbf{v} \cdot \nabla \omega \right] = \nabla^2 \omega - \text{Ra} \frac{\partial T}{\partial x}$$

$$\nabla^2 \psi = -\omega$$

$$\mathbf{v} = \nabla \times \psi \mathbf{k}, \quad \omega = (\nabla \times \mathbf{v}) \cdot \mathbf{k}$$

$$\text{Ra} = \frac{\alpha \Delta T g d^3}{\nu \kappa}, \quad \text{Pr} = \frac{\nu}{\kappa}$$

## The Lorenz Equations and chaos

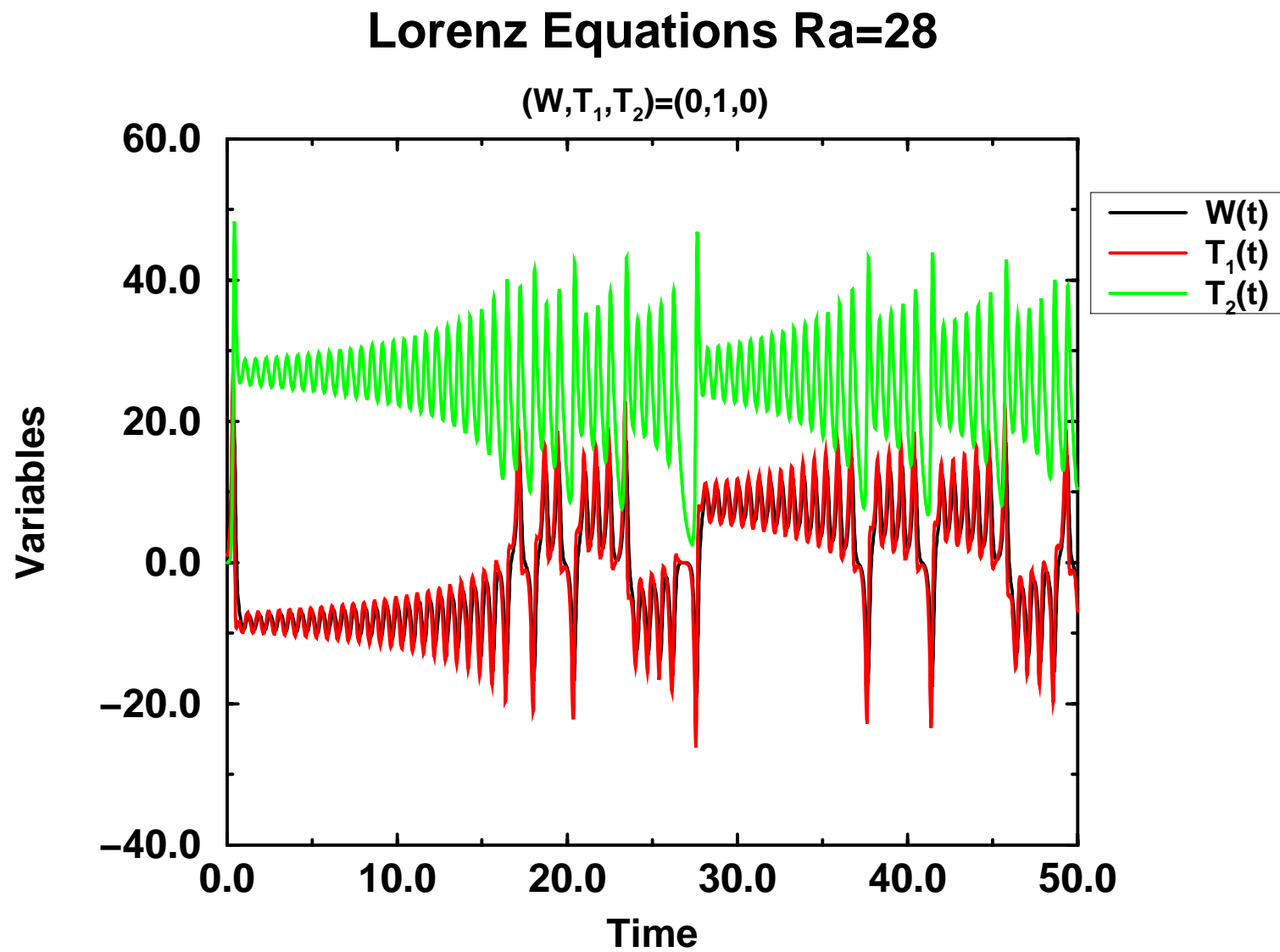
Let

$$\psi(t, \mathbf{x}) = W(t) \sin(a\pi x) \sin(\pi z)$$

$$T(t, \mathbf{x}) = (1 - z) + T_1(t) \cos(a\pi x) \sin(\pi z) + T_2(t) \sin(2\pi z)$$

Then RB convection becomes

$$\begin{aligned}\frac{dW}{dt} &= \text{Pr}(T_1 - W) \\ \frac{dT_1}{dt} &= -WT_2 + rW - T_1 \\ \frac{dT_2}{dt} &= WT_1 - bT_2\end{aligned}$$



# Linearized Shallow water equations

equatorial  $\beta$  plane

$$\frac{\partial \mathbf{v}}{\partial t} + \beta y \mathbf{k} \times \mathbf{v} = -g \nabla \eta$$

$$\frac{\partial \eta}{\partial t} + \nabla \cdot (H \mathbf{v}) = 0$$

With forcing and dissipation (ala Cane-Zebiak)

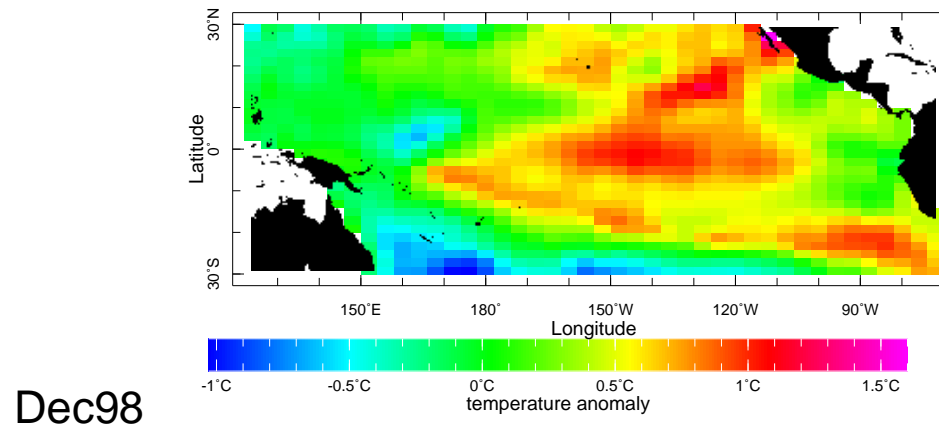
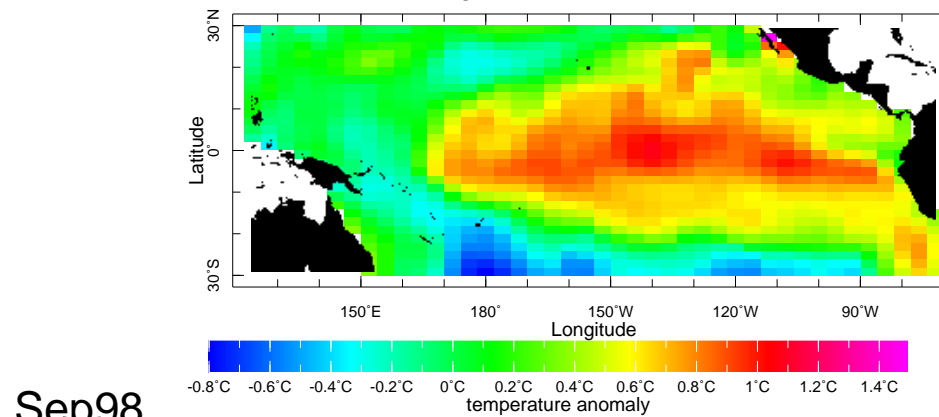
$$\frac{\partial \mathbf{v}}{\partial t} + \beta y \mathbf{k} \times \mathbf{v} = -g H_0 \nabla \eta + \boldsymbol{\tau} / \rho - r \mathbf{v}$$

$$\frac{\partial \eta}{\partial t} + \nabla \cdot (H \mathbf{v}) = -r \eta$$

# Sea Surface temperature anomalies

## LDEO2 El Niño model

Sea Surface temperature anomalies

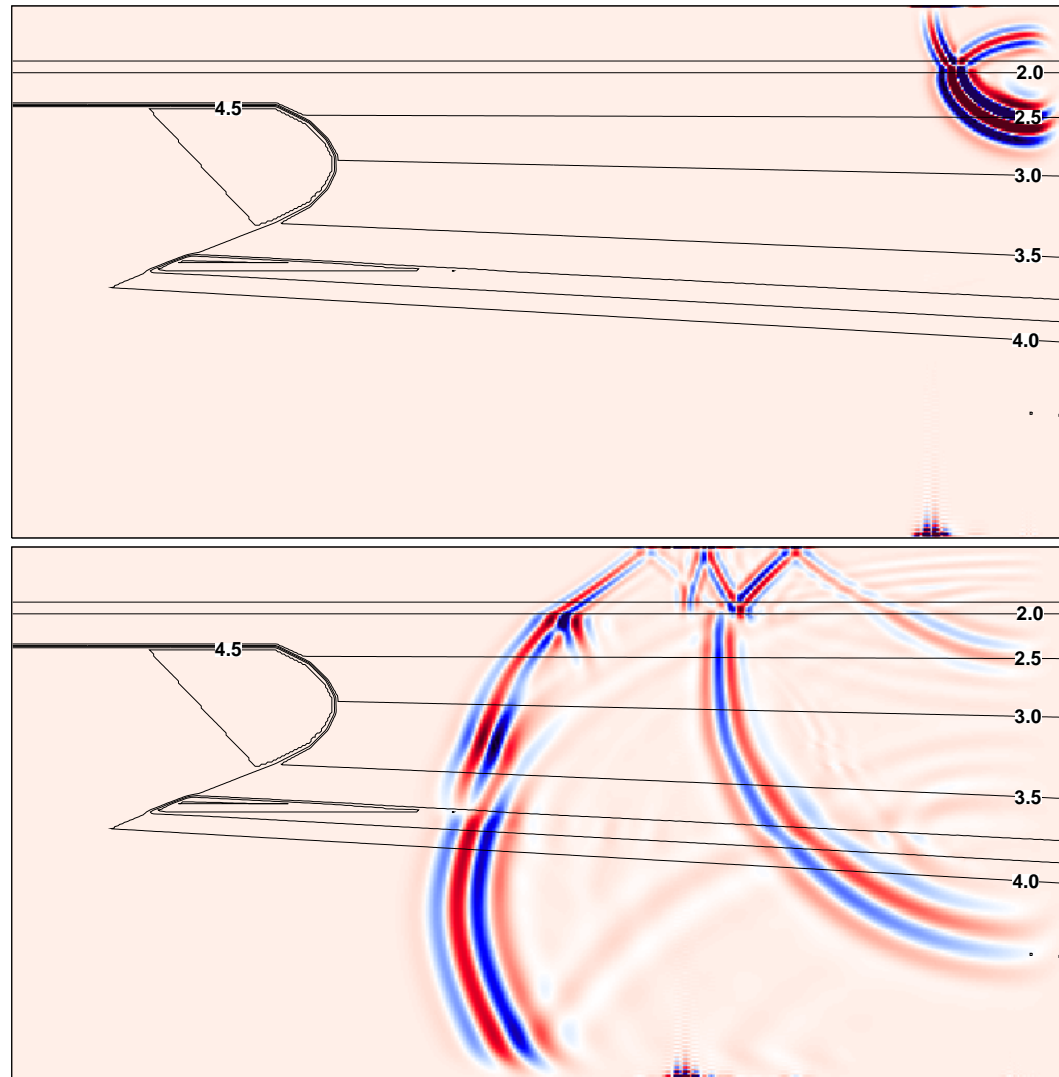


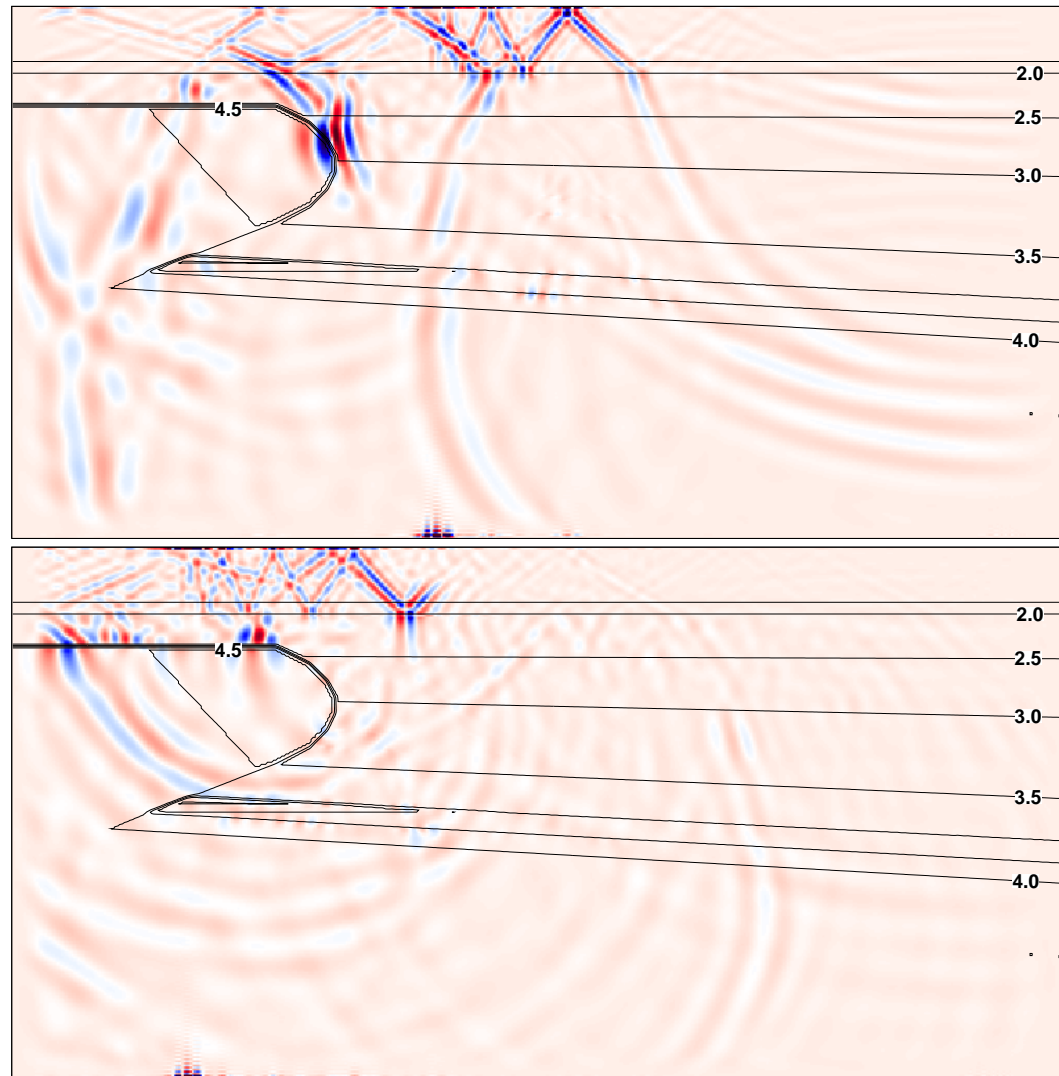
## Seismic Wave propagation

$$\rho \frac{\partial \mathbf{v}}{\partial t} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f}$$

$$\frac{\partial \sigma_{ij}}{\partial t} = \mu \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \lambda \nabla \cdot \mathbf{v} \delta_{ij}$$

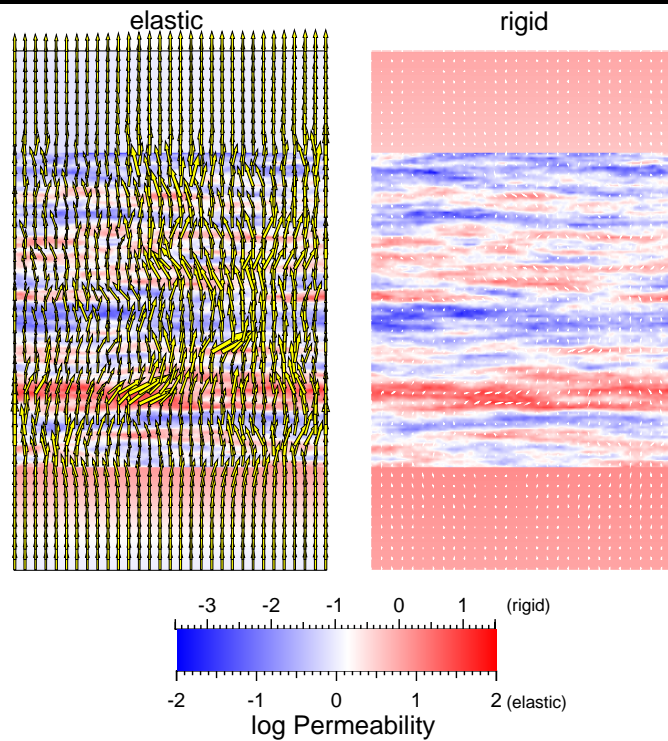
Solutions by Pseudo-spectral techniques ala Gustavo Correa (LDEO)





## Flow in heterogeneous porous media

$$\nabla \cdot \frac{K}{\mu} [\nabla P - \rho_f \mathbf{g}] = 0$$



## Flow in deformable porous media (magma migration)

$$\frac{\partial(\rho_f \phi)}{\partial t} + \nabla \cdot (\rho_f \phi \mathbf{v}) = \Gamma$$

$$\frac{\partial[\rho_s(1 - \phi)]}{\partial t} + \nabla \cdot [\rho_s(1 - \phi)\mathbf{v}] = -\Gamma$$

$$\phi(\mathbf{v} - \mathbf{v}) = \frac{-k_\phi}{\mu} [\nabla P - \rho_f \mathbf{g}]$$

$$\nabla P = -\nabla \times [\eta \nabla \times \mathbf{v}] + \nabla [(\zeta + 4\eta/3) \nabla \cdot \mathbf{v}] + \mathbf{G} - \bar{\rho} \mathbf{g}$$

$$k_\phi \sim \frac{a^2 \phi^n}{b}$$

## Flow in deformable porous media (2-D potential form, non-dimensional)

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = (1 - \phi_0 \phi) \mathcal{C} + \Gamma$$

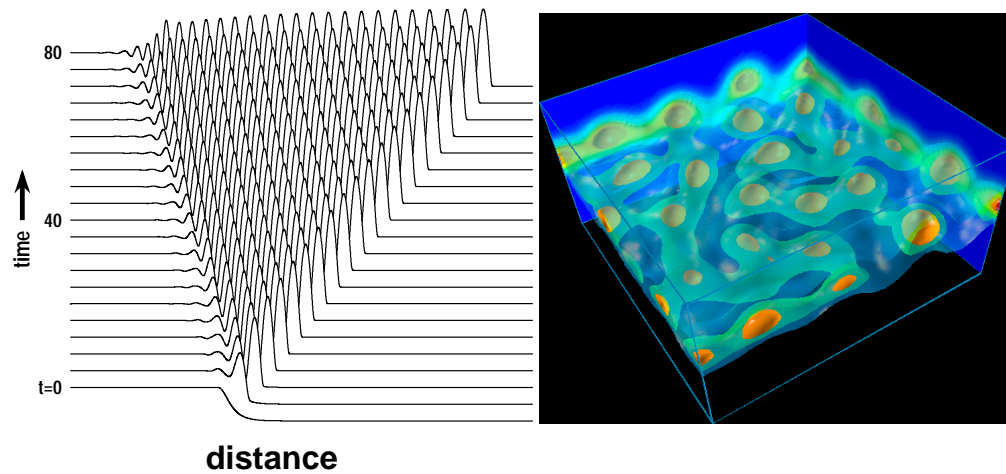
$$-\nabla \cdot k_\phi \nabla \mathcal{C} + \mathcal{C} = \nabla \cdot k_\phi [-\nabla \times \omega \mathbf{j} - (1 - \phi_0 \phi) \mathbf{k}] + \Gamma \frac{\delta \rho}{\rho_f}$$

$$\nabla^2 \mathcal{U}^s = \mathcal{C}$$

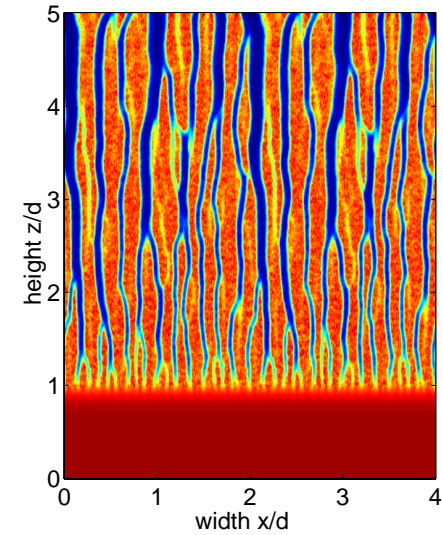
$$\nabla^2 \omega = -\frac{g}{\eta} \frac{\partial \rho}{\partial x}$$

$$\nabla^2 \psi^s = -\omega$$

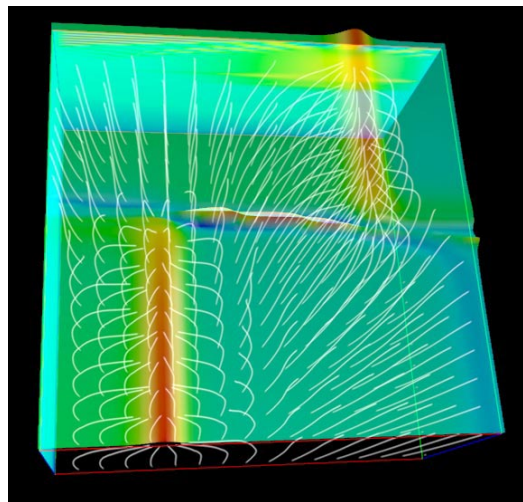
### Non-linear Porosity waves



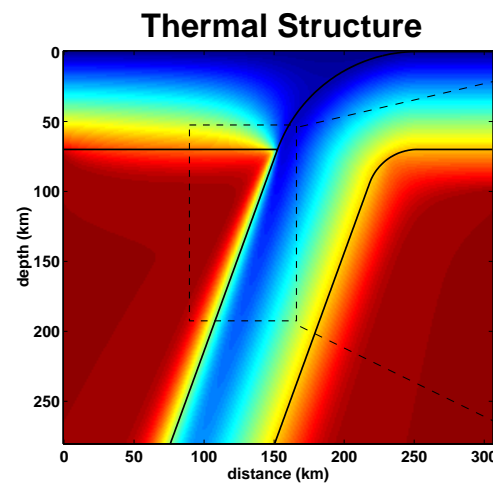
### Reactive Flow Localization



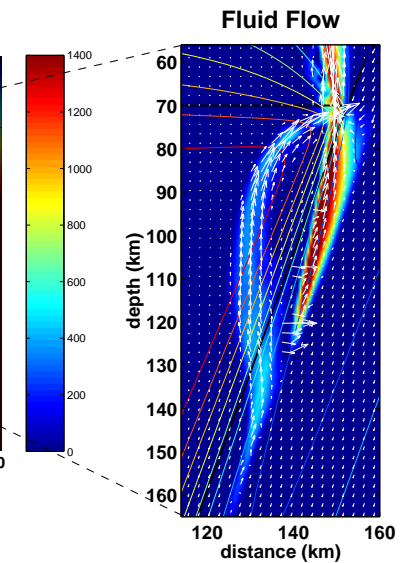
### Earth Science Applications



mid-ocean ridges



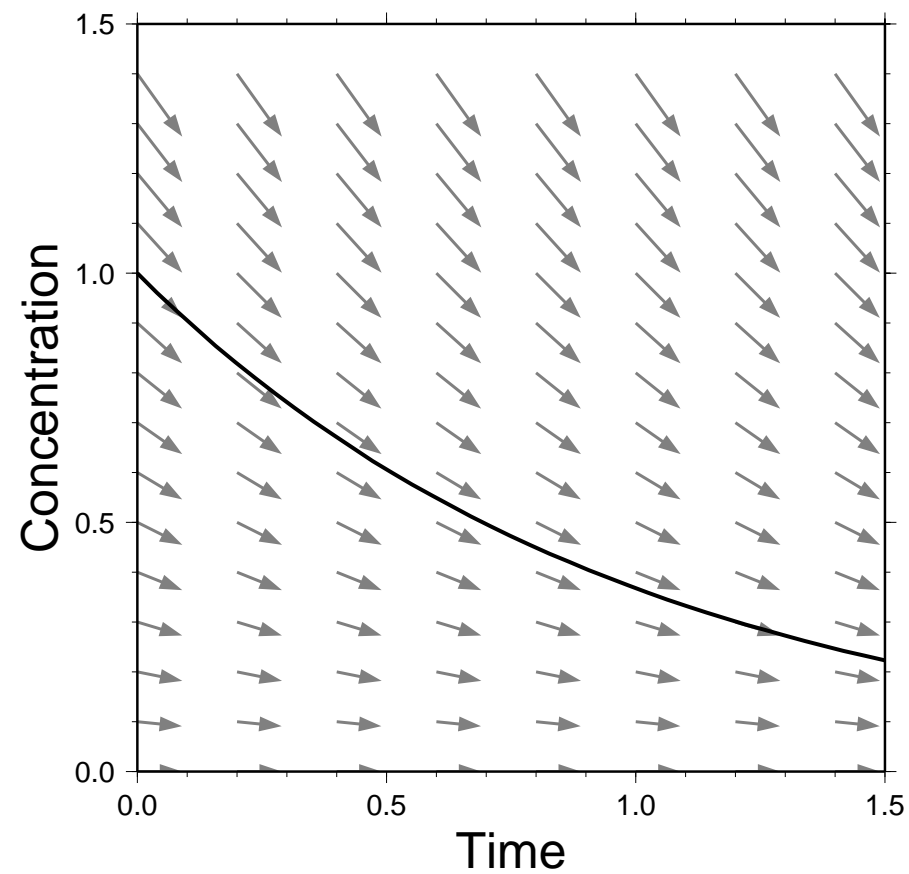
subduction zones



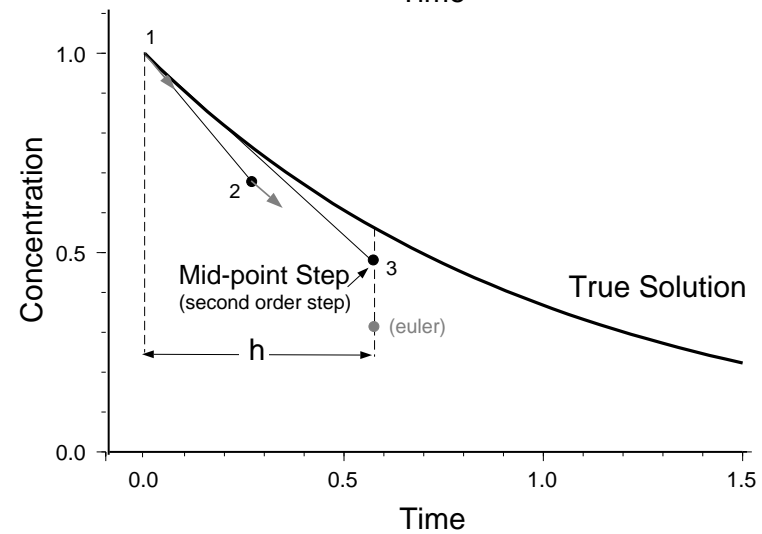
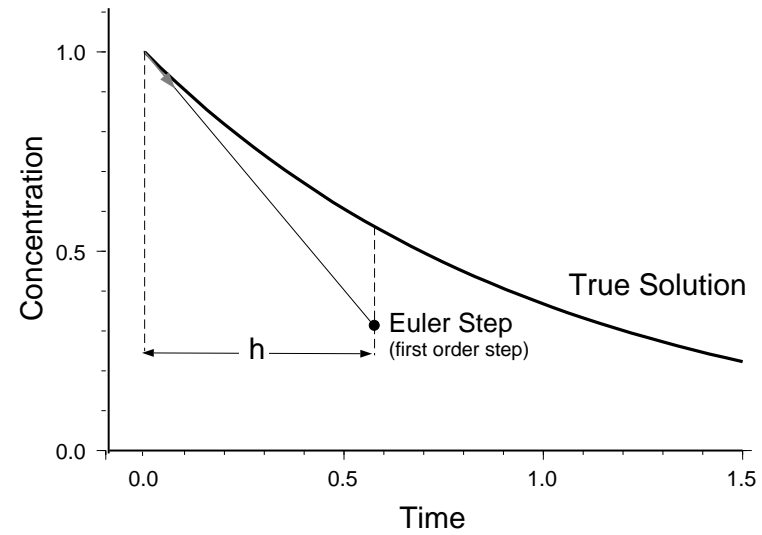
Fluid Flow

## Direction fields and solutions for

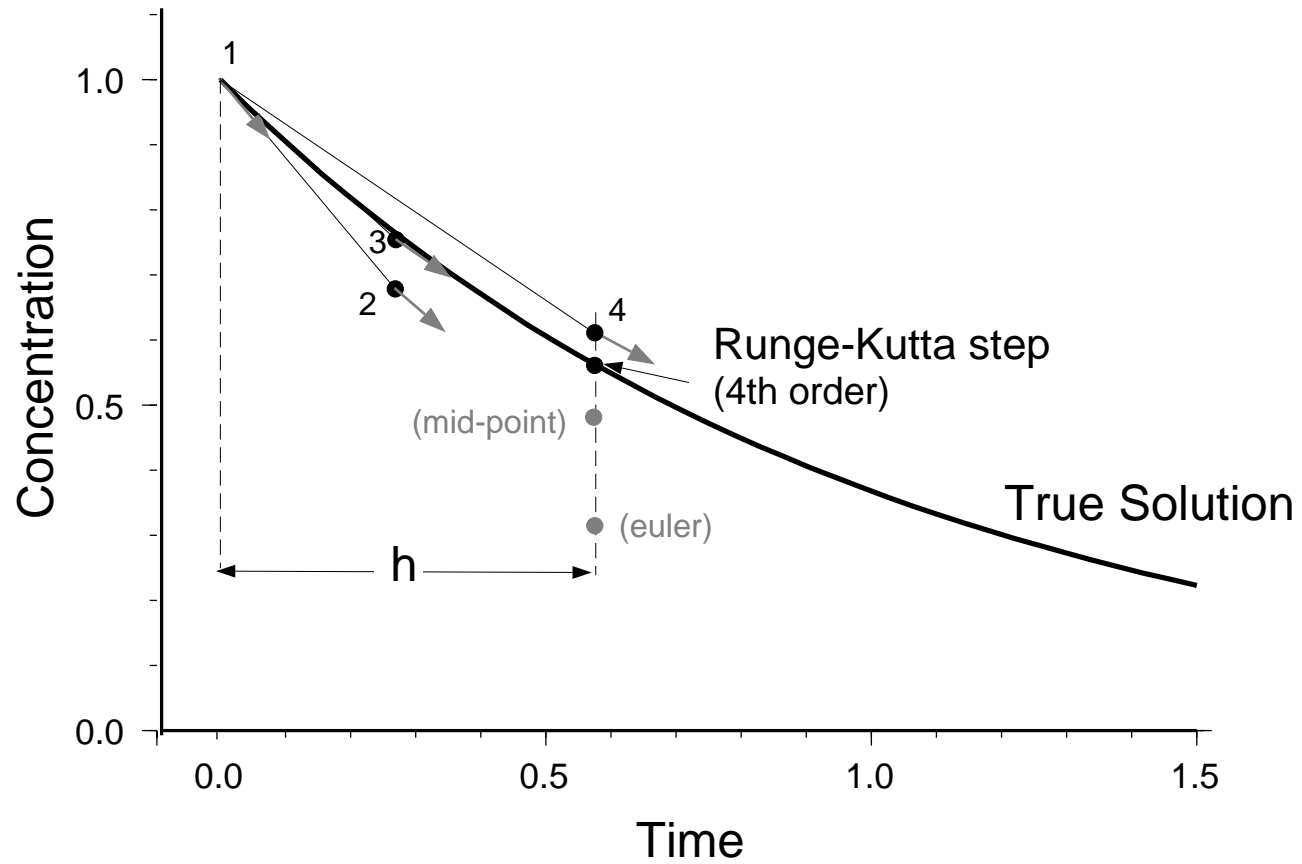
$$\frac{dc}{dt} = -c$$



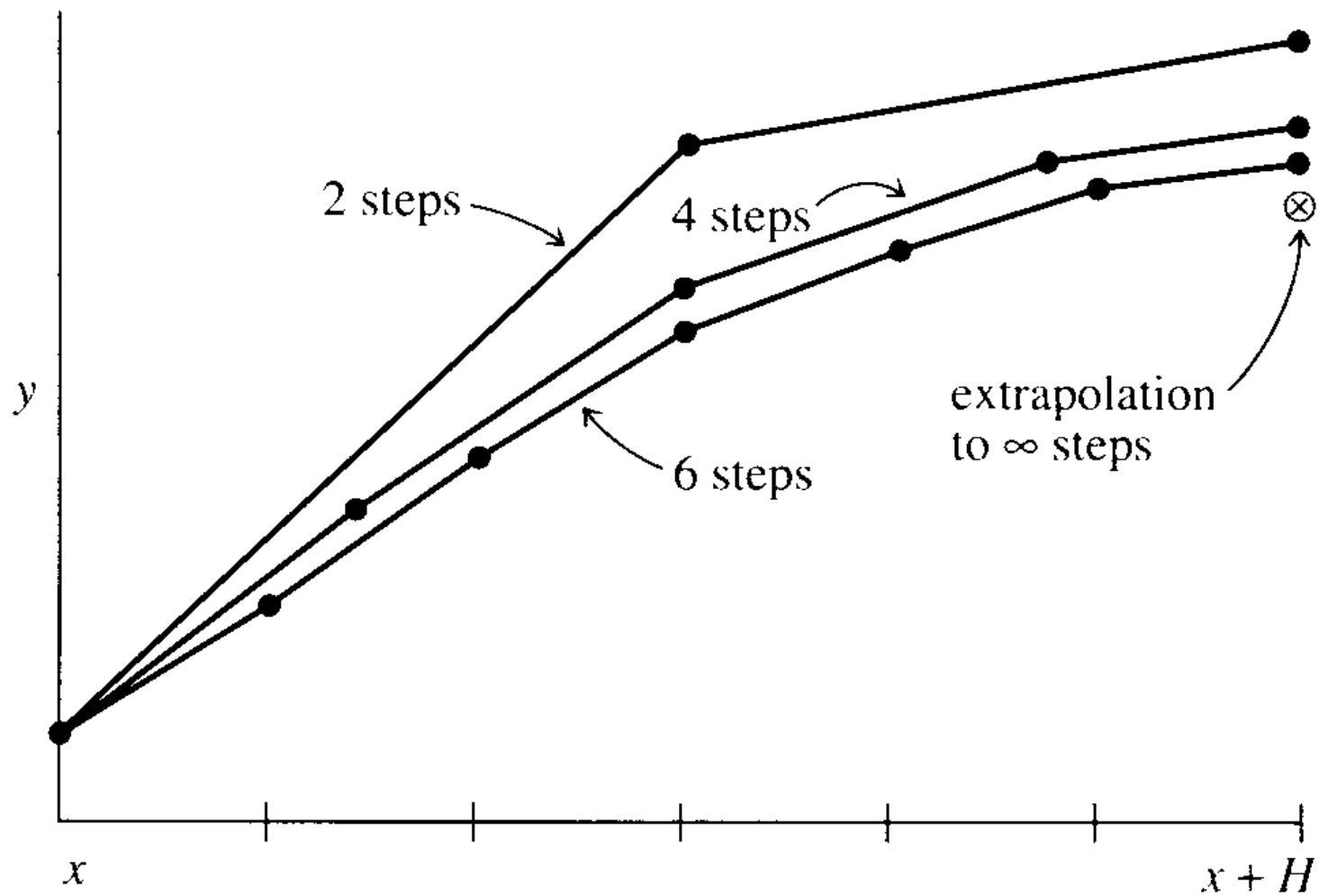
## Simple Stepping Schemes



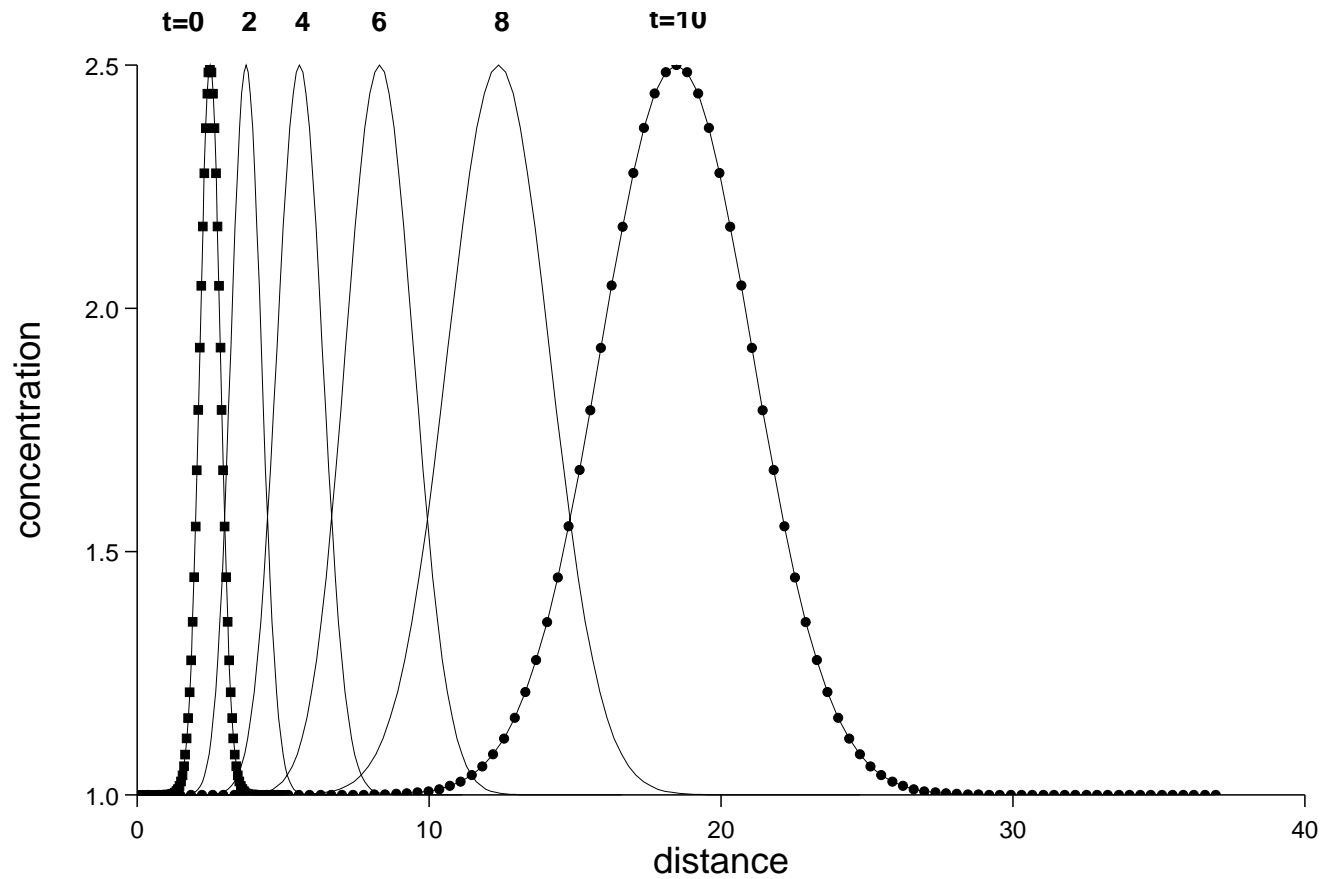
### 4th Order Runge-Kutta Step



## Bulirsch-Stoer Stepping using Richardson Extrapolation

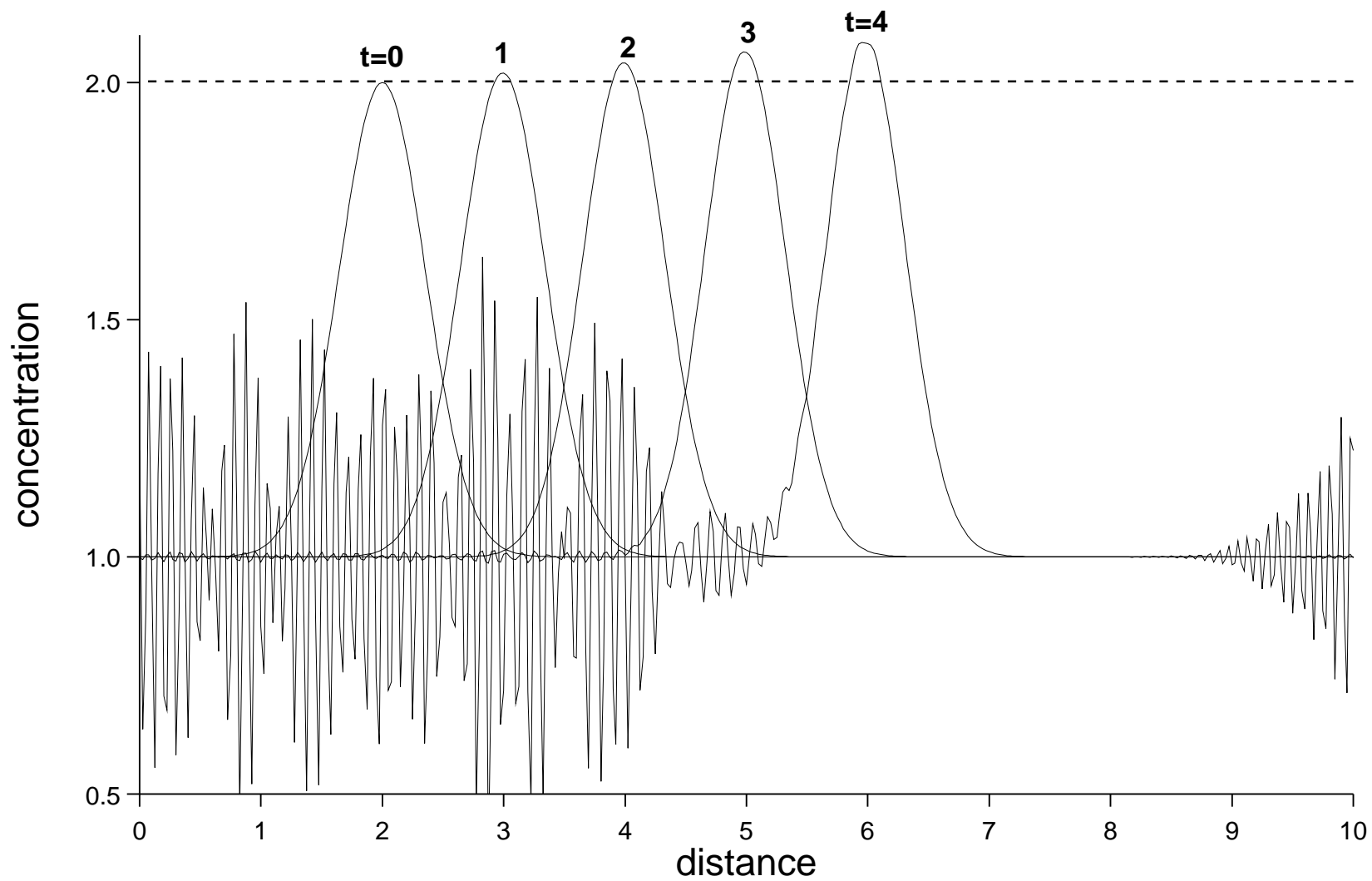


## Transport by Characteristics: Particle based methods



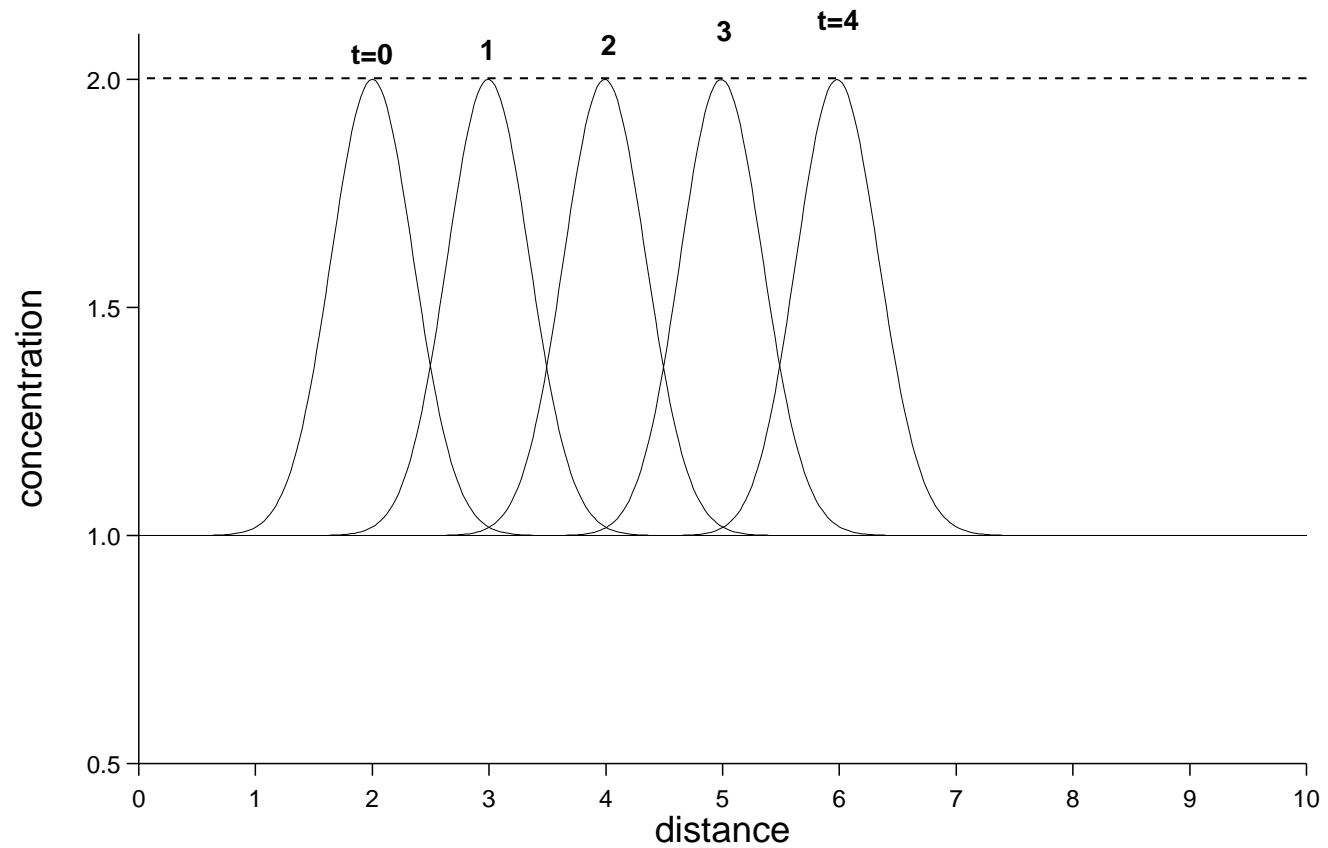
$$v(x) = 0.2x$$

# FTCS Explodes!

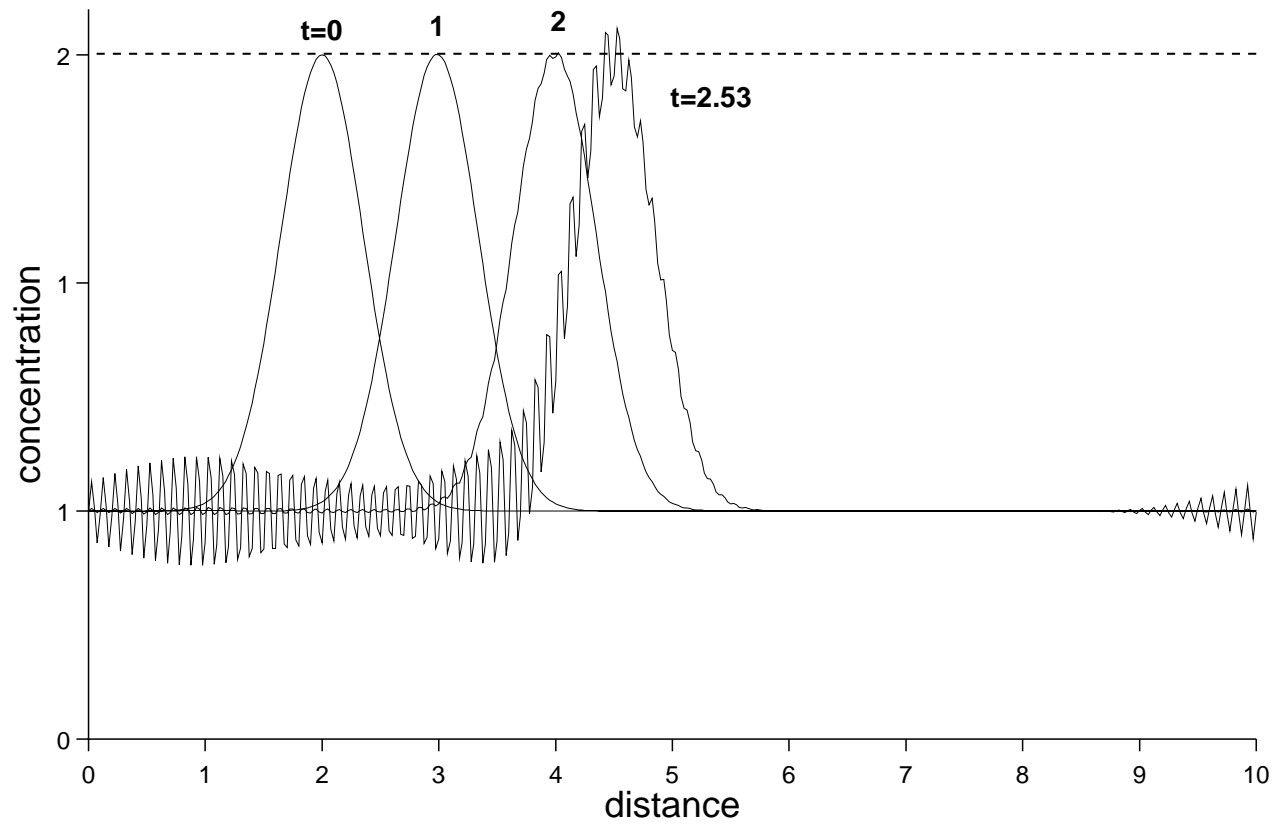


## Staggered Leapfrog works ( $\alpha < 1$ )

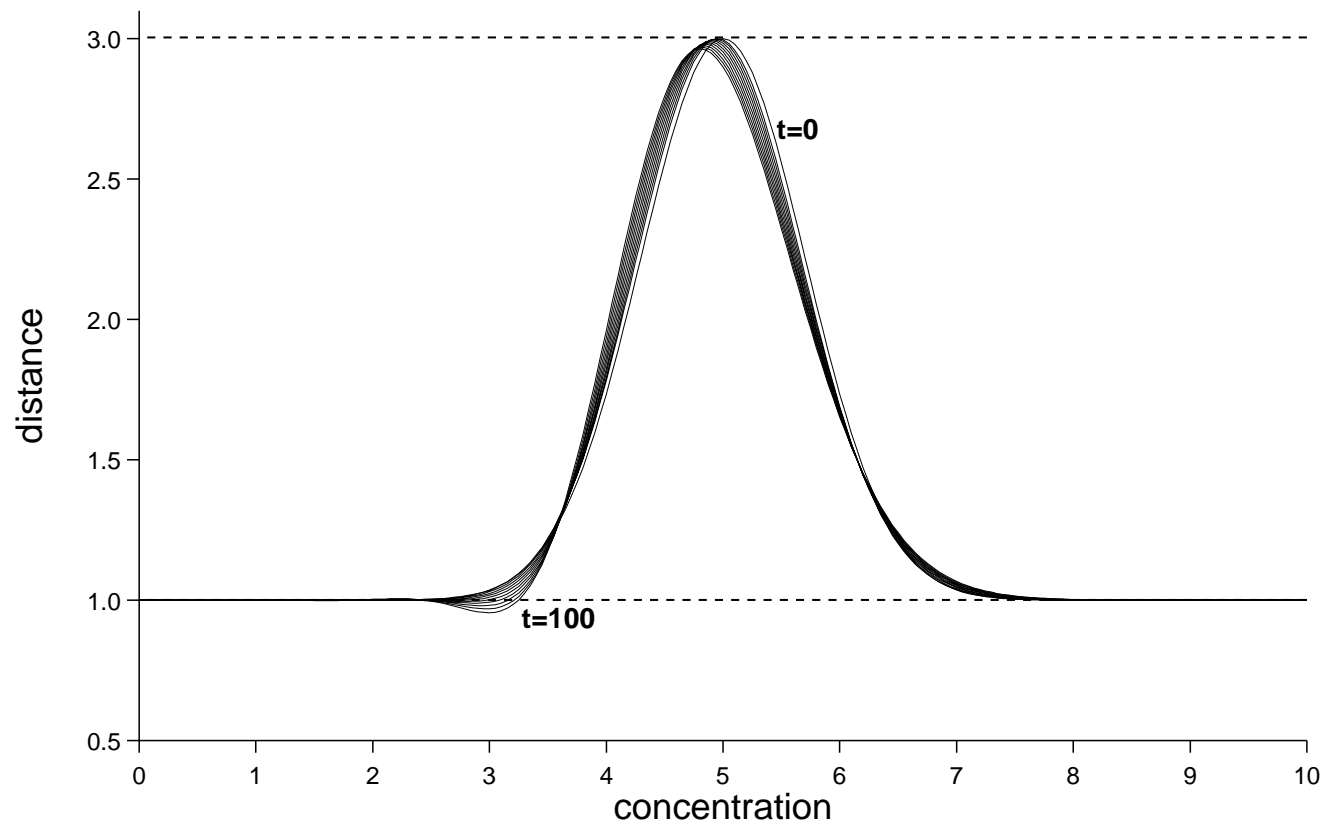
$$\alpha = 0.9$$

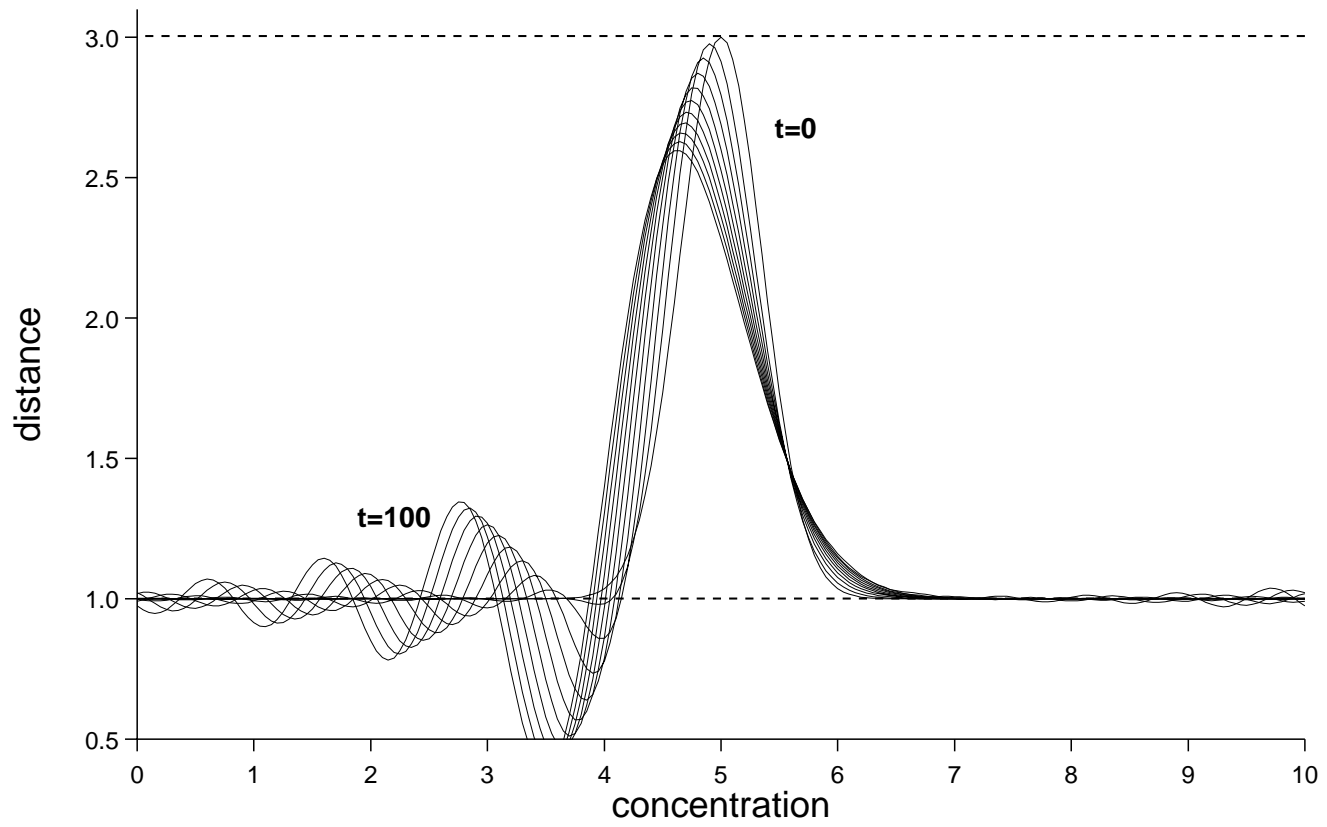


$$\alpha = 1.01$$

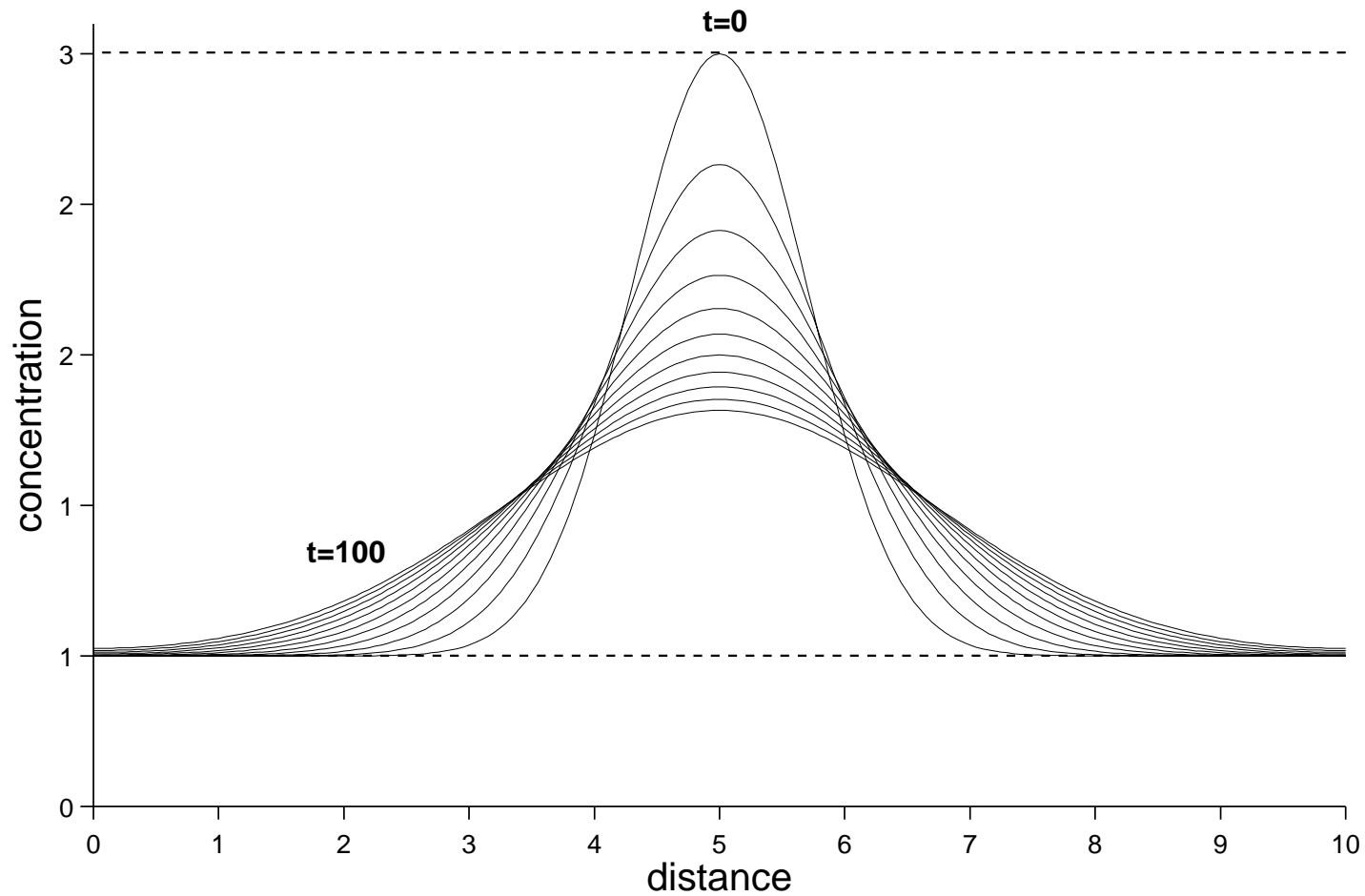


## Staggered Leapfrog disperses ( $\alpha = 0.5$ )

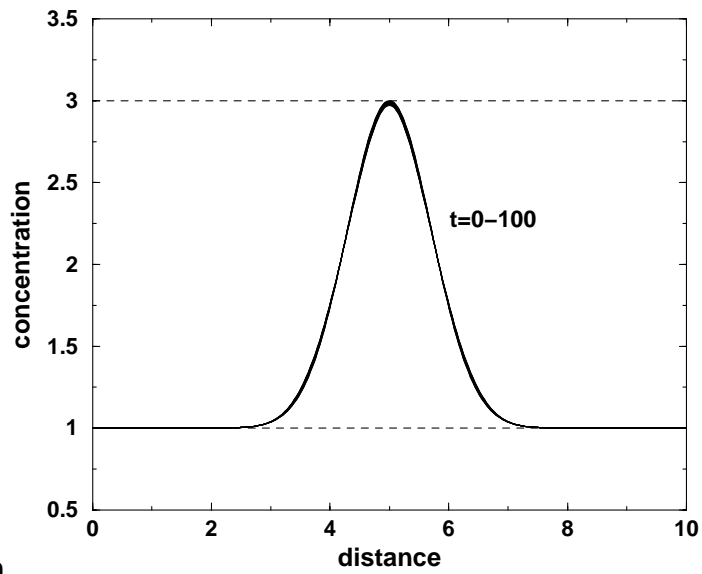




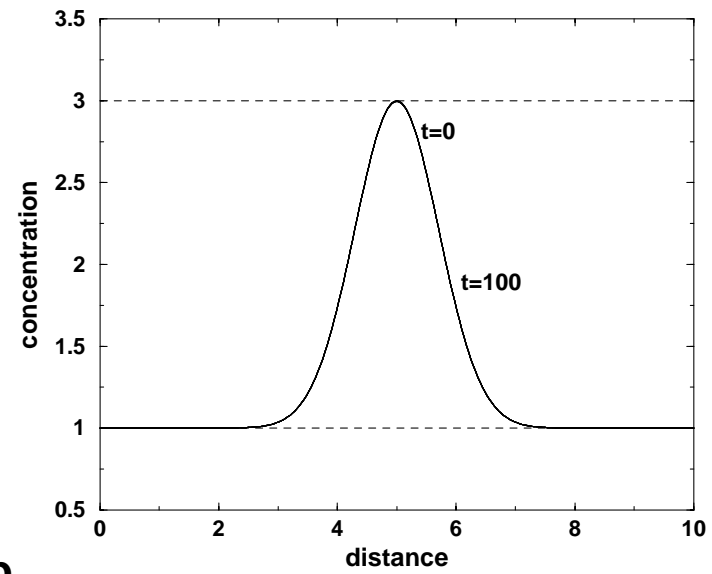
## Simple Upwind diffuses (badly) ( $\alpha = 0.5$ )



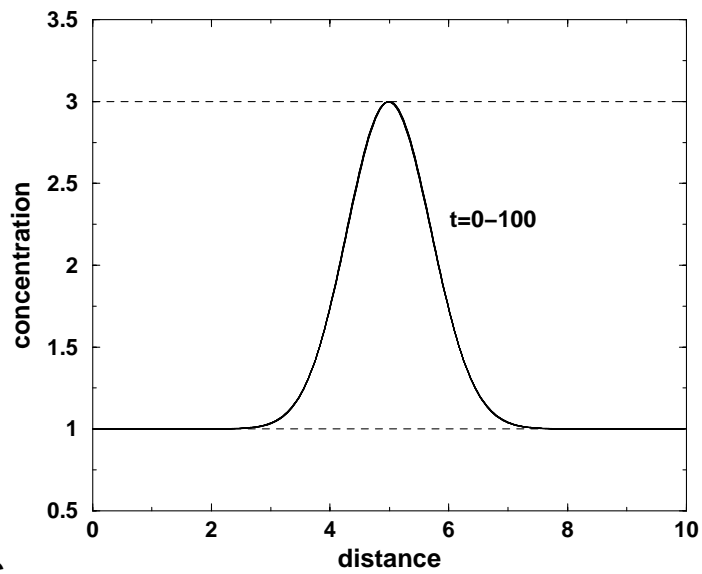
## Better schemes



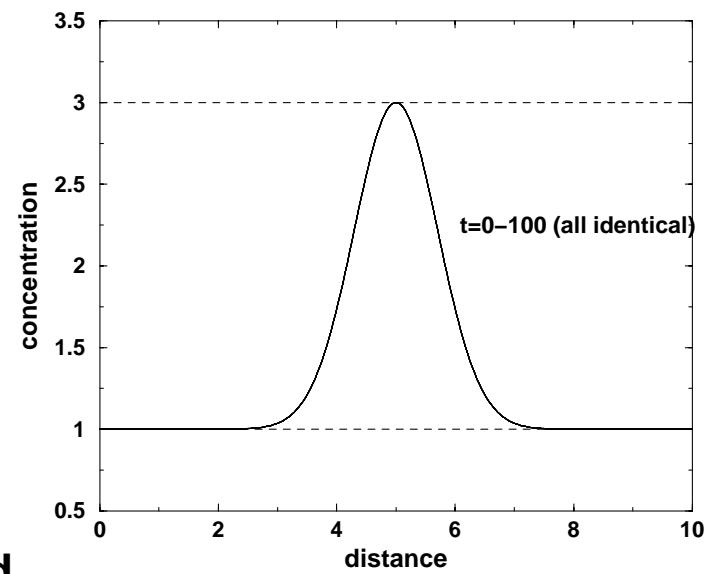
**a**



**b**

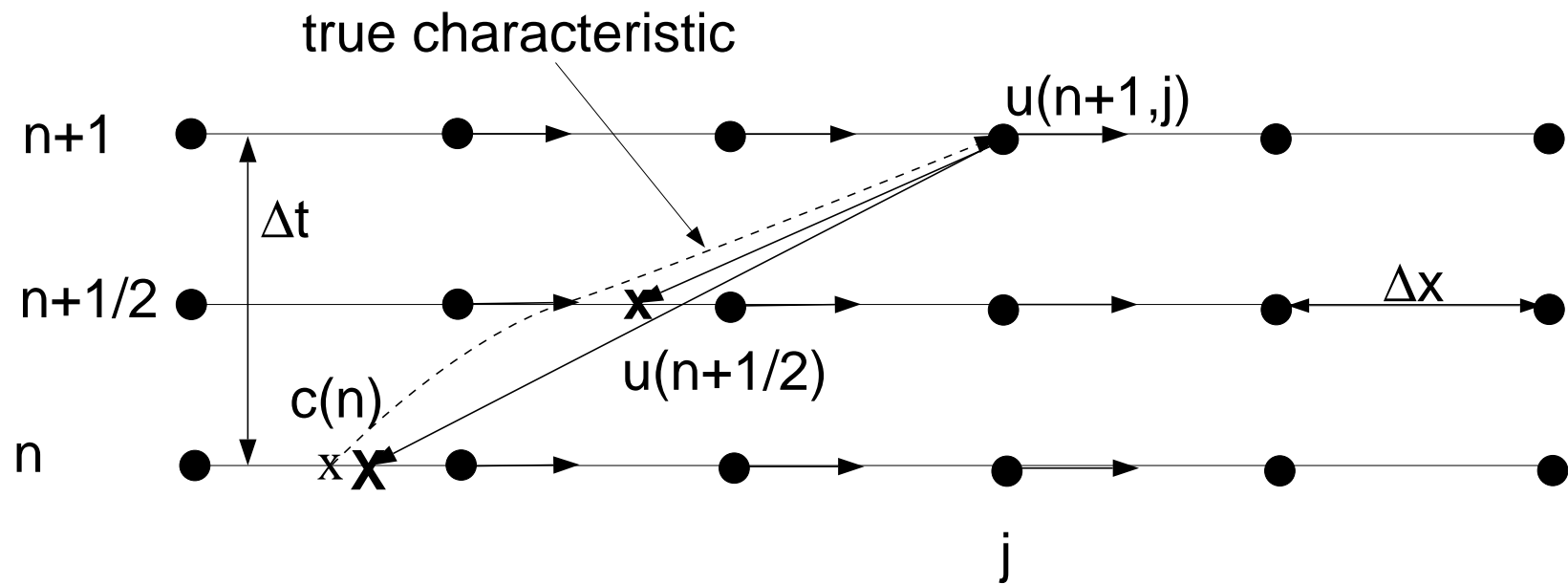


**c**

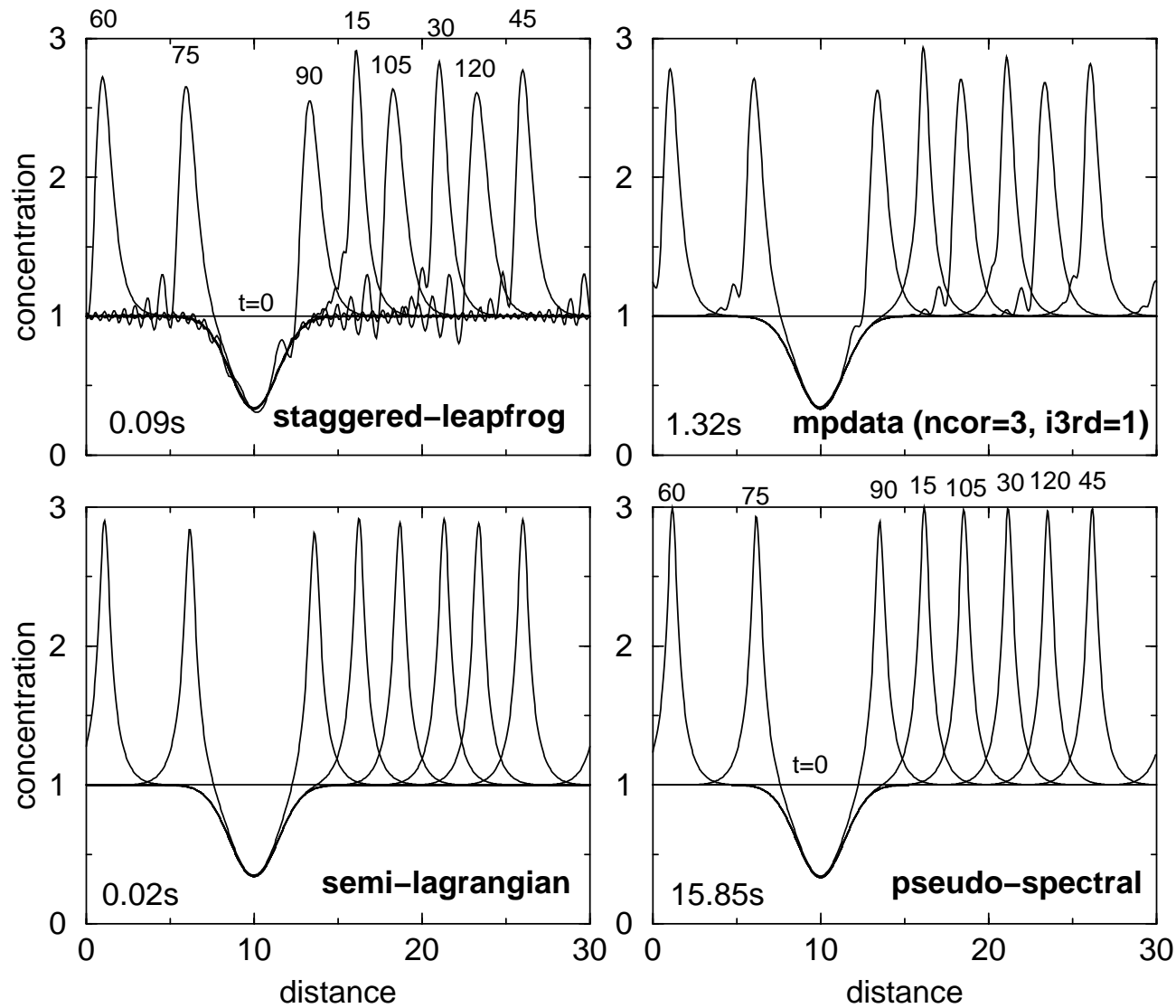


**d**

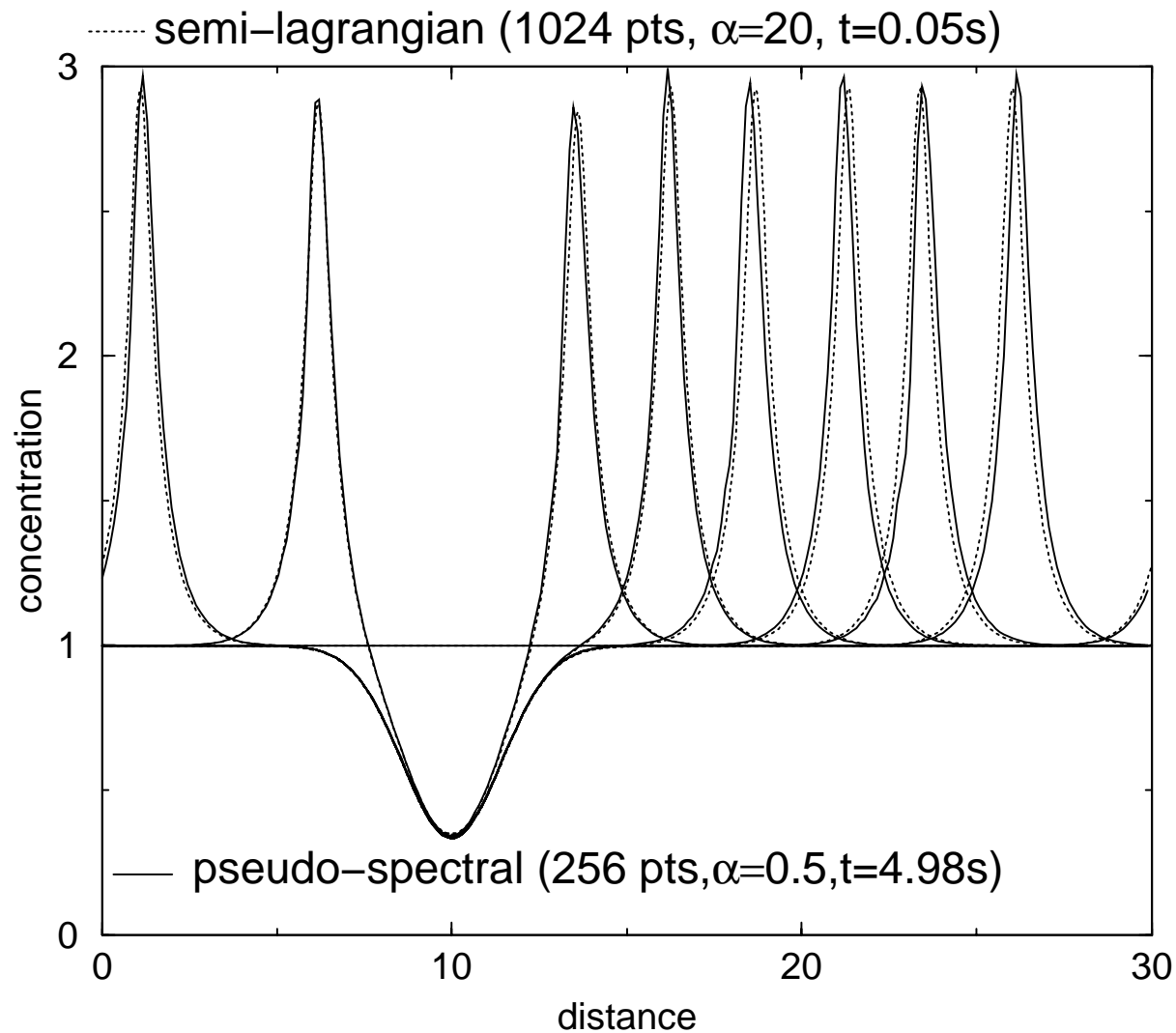
## Semi-Lagrangian Schemes: a recipe



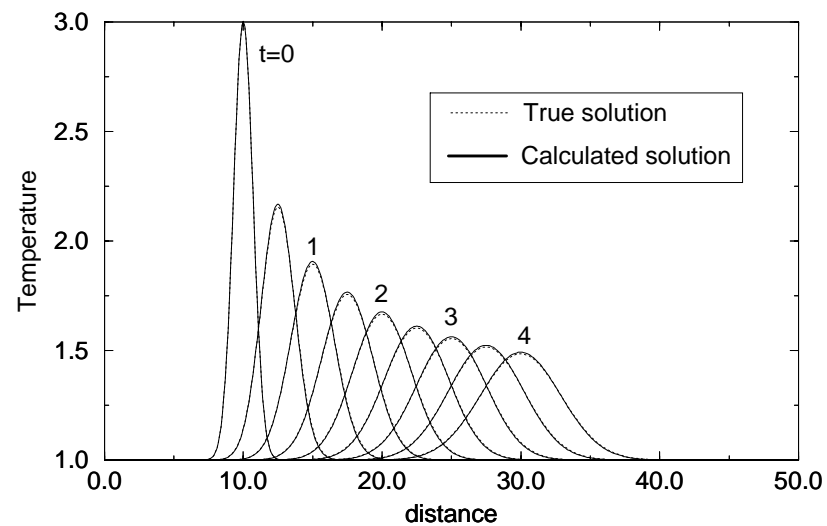
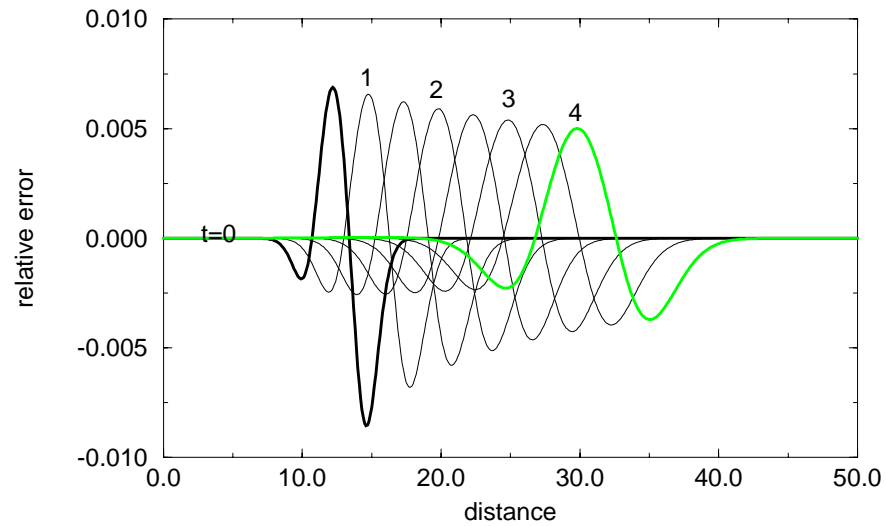
## Behaviour with non-constant velocity



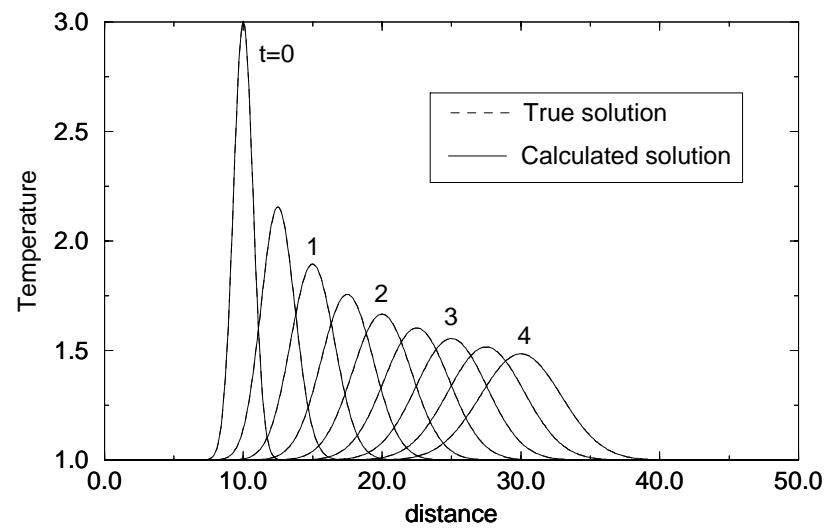
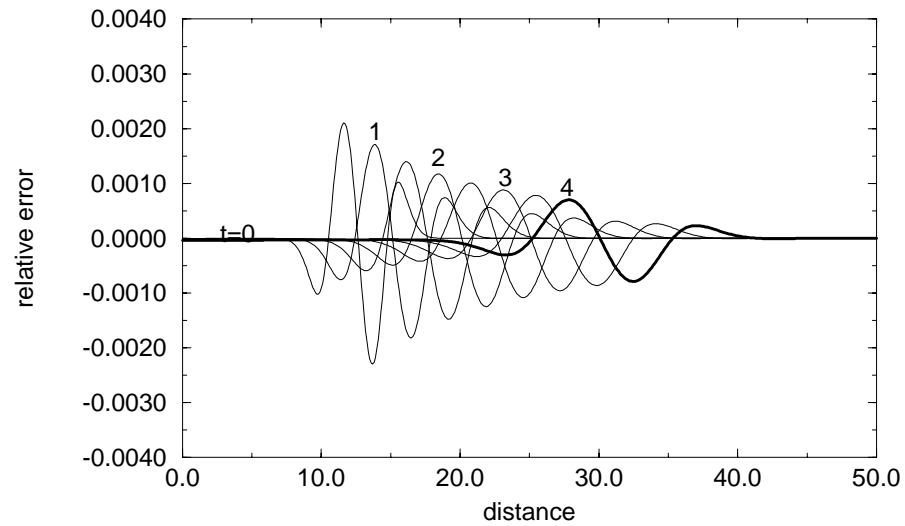
## Comparison of Pseudo-spectral and Semi-Lagrangian schemes



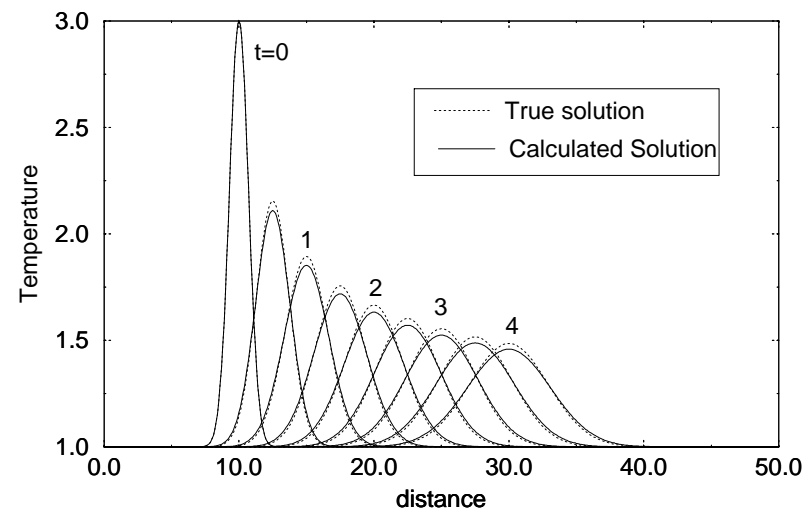
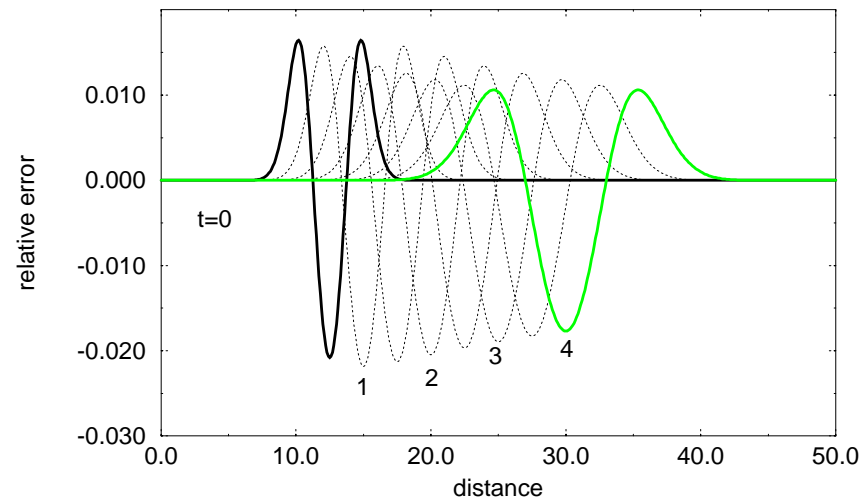
# Advection-diffusion: FTCS



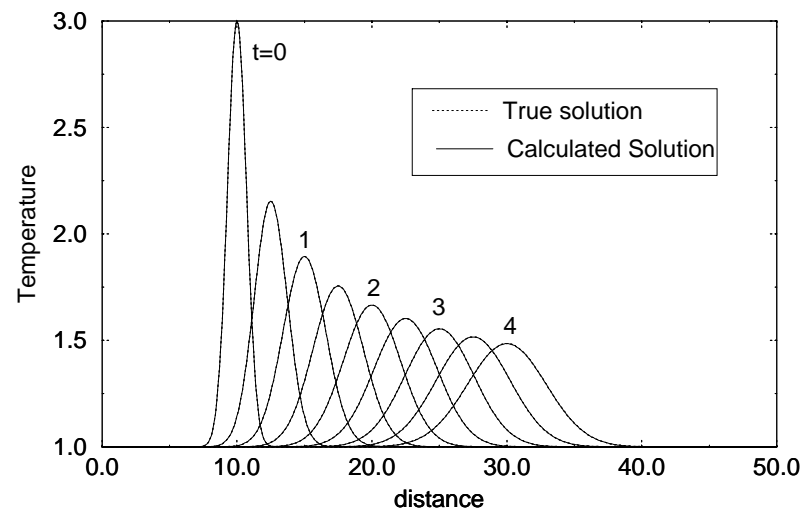
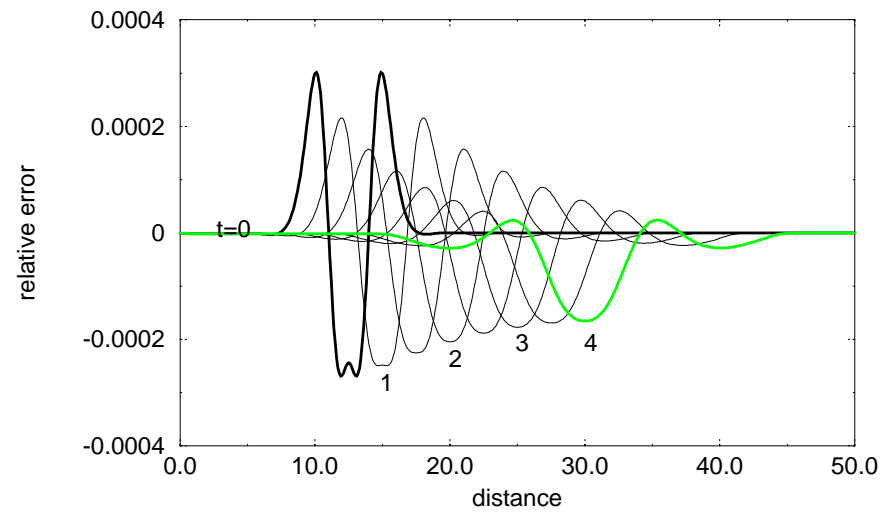
# Advection-diffusion: Crank-Nicholson



## Advection-diffusion: Operator-Splitting MPDATA + CN (no corrections... upwind scheme)

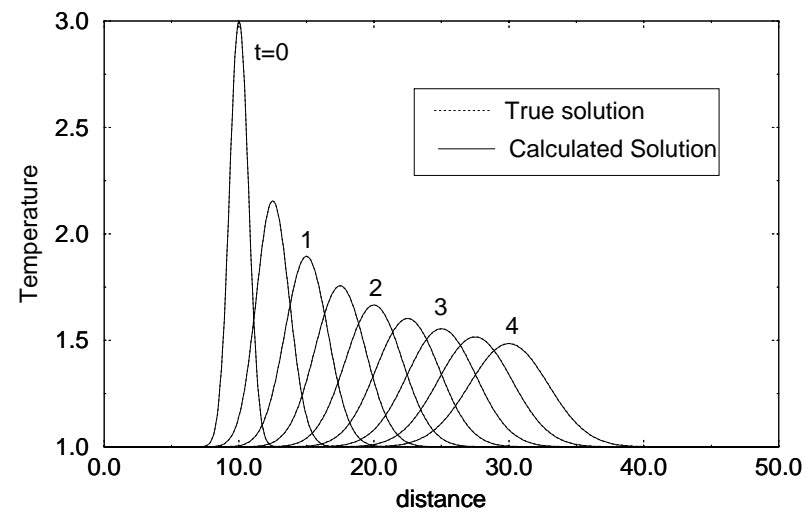
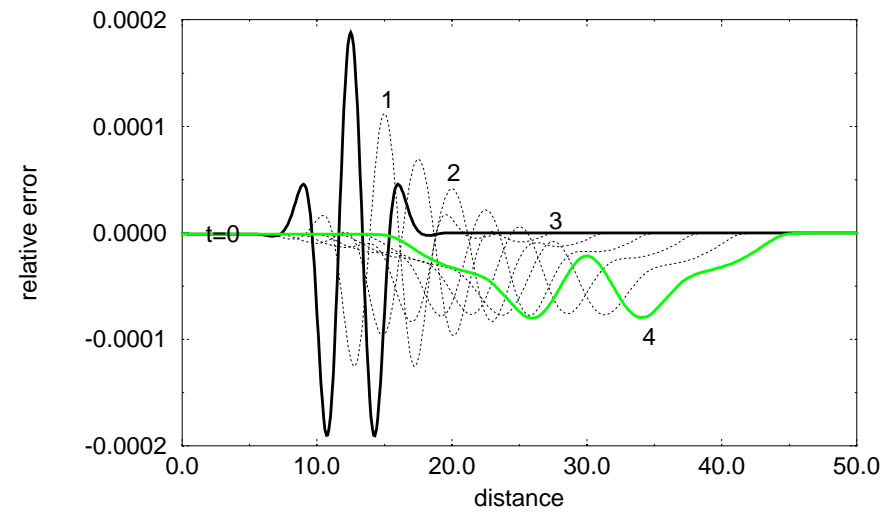


## Advection-diffusion: Operator-Splitting MPDATA + CN (one correction)



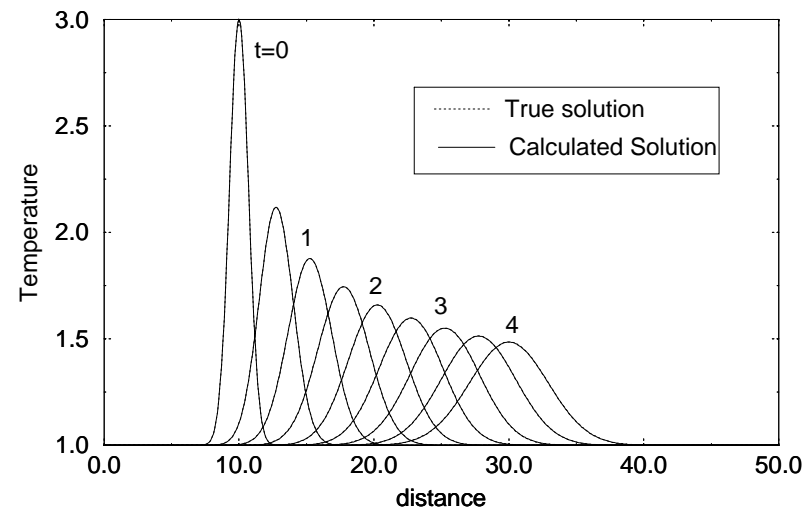
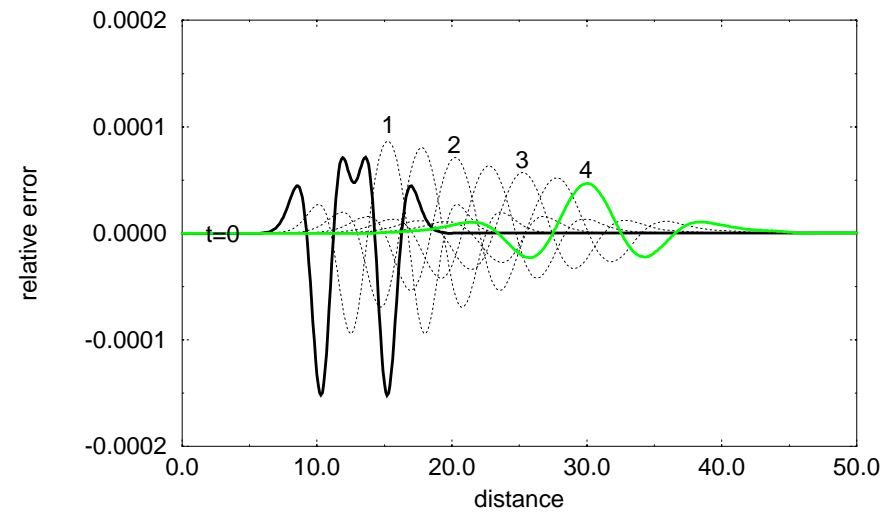
# Advection-diffusion: Operator-Splitting MPDATA + CN

## Da Woiks! (ncor=3, i3rd=1)



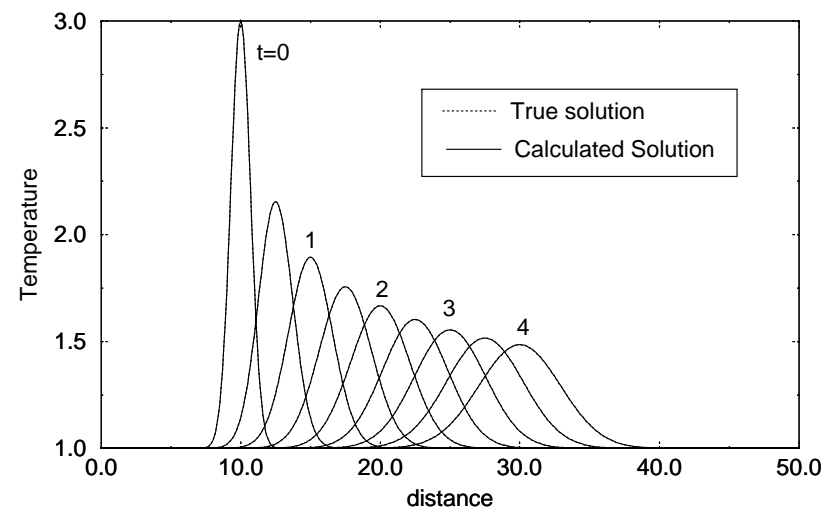
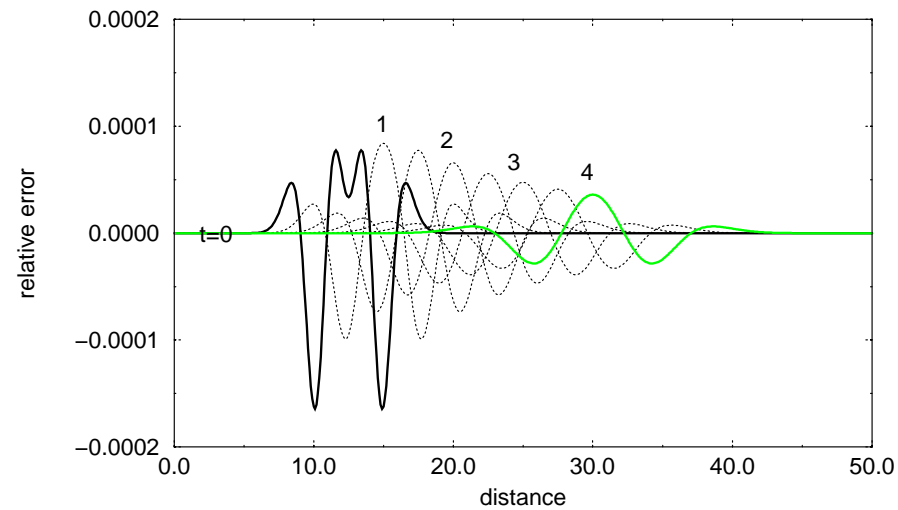
# Advection-diffusion: Operator-Splitting Semi-Lagrangian + CN

$$\alpha = 2.5$$

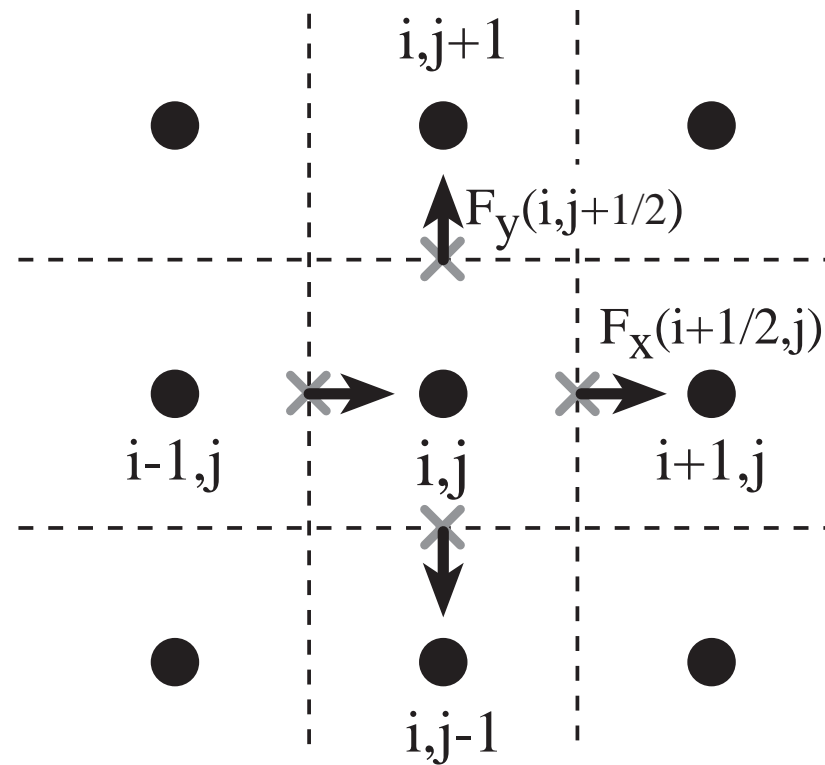


## Advection-diffusion: All-in-one Semi-LagrangianCN

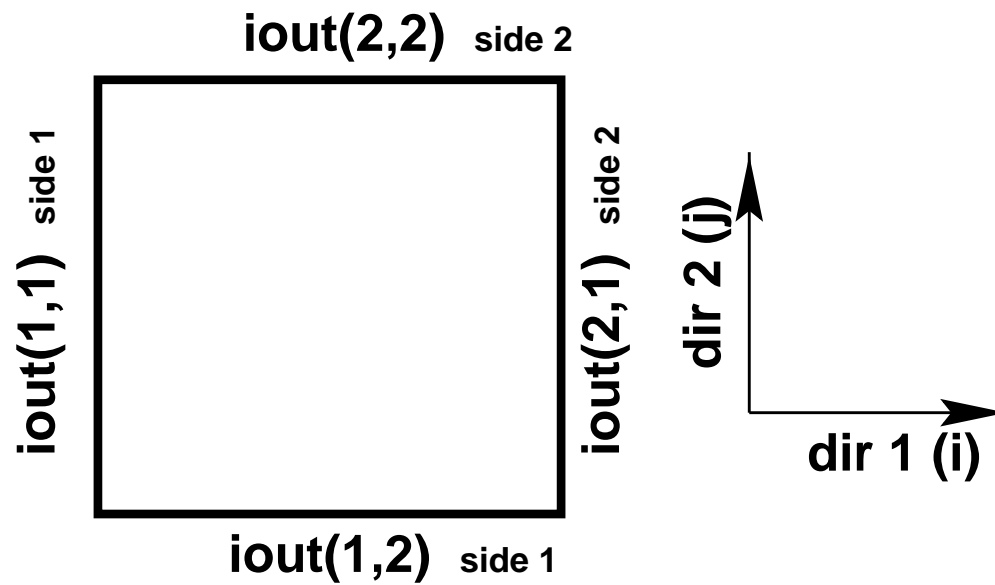
$$\alpha = 2.5$$



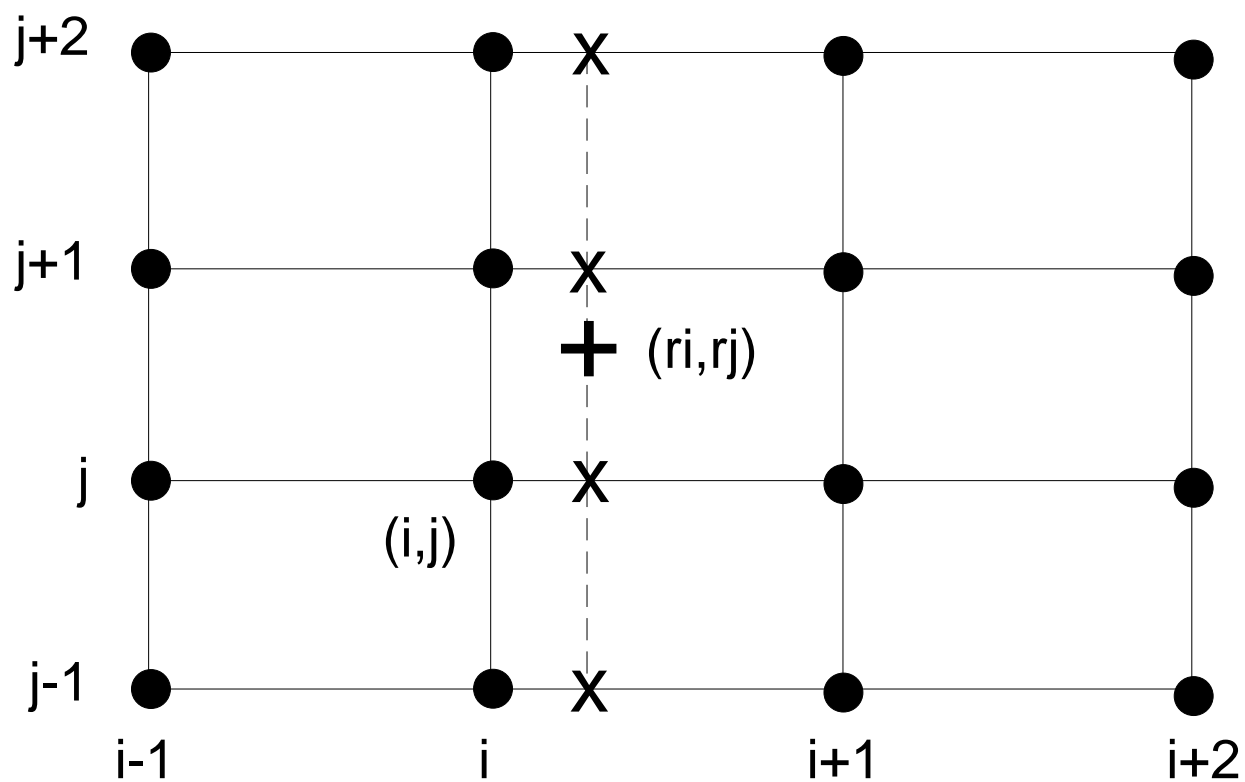
## 2-D control volume



## Boundary condition pointers

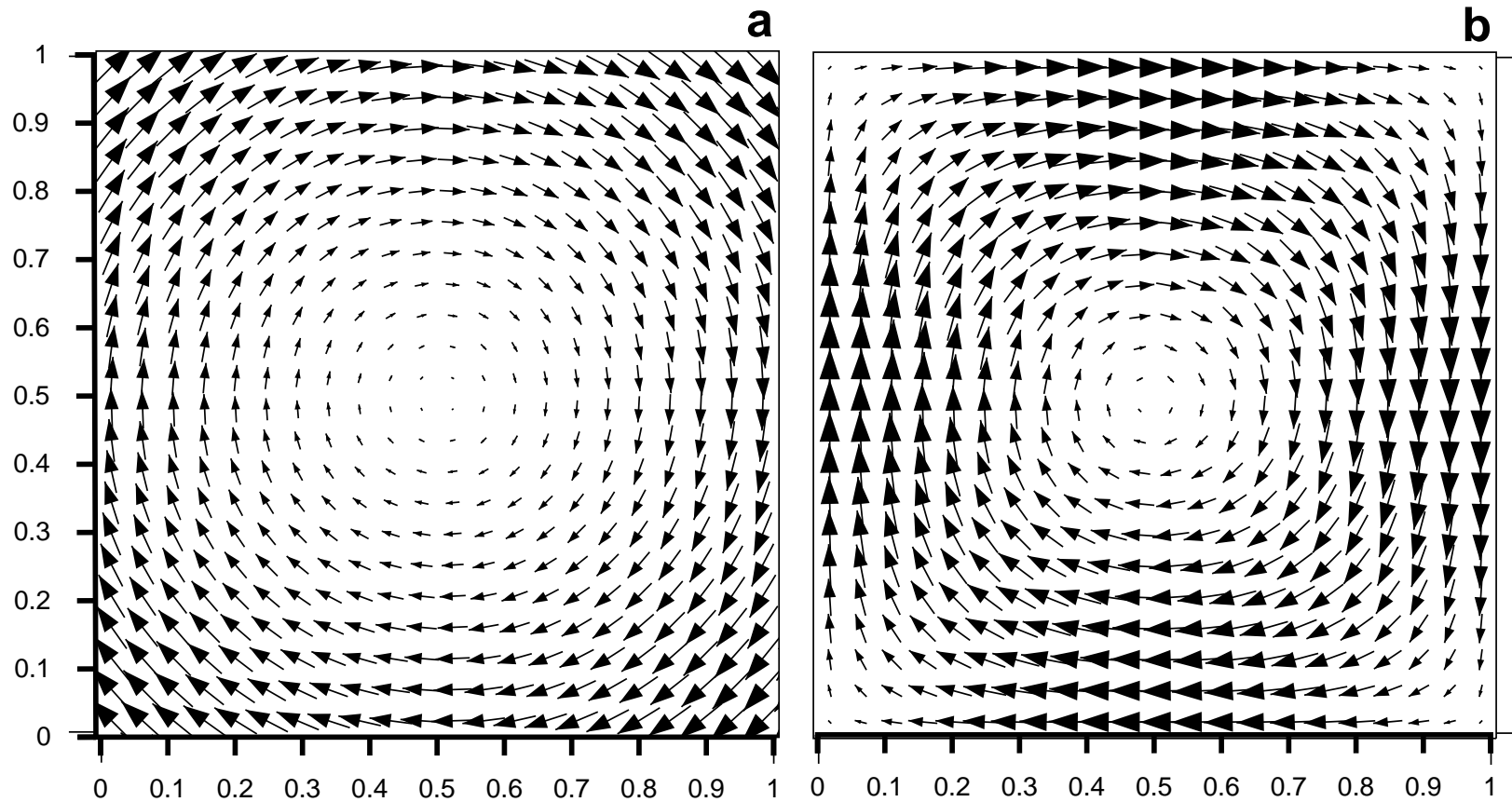


## Bicubic interpolation

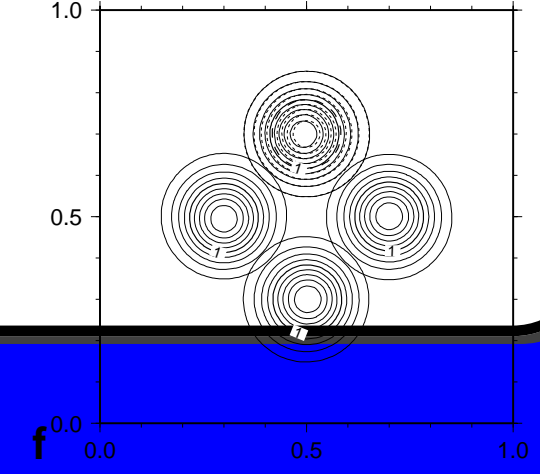
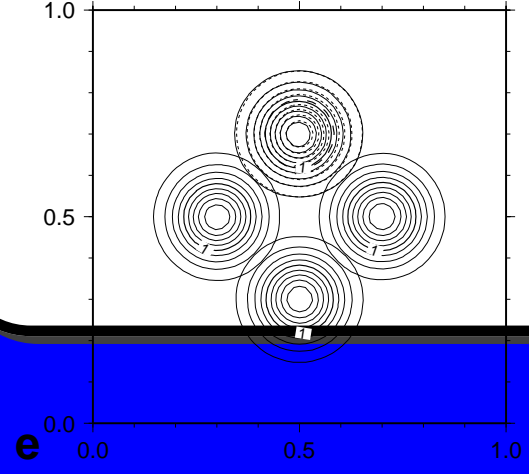
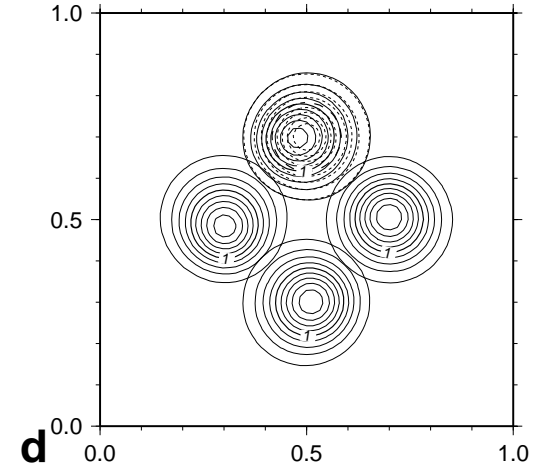
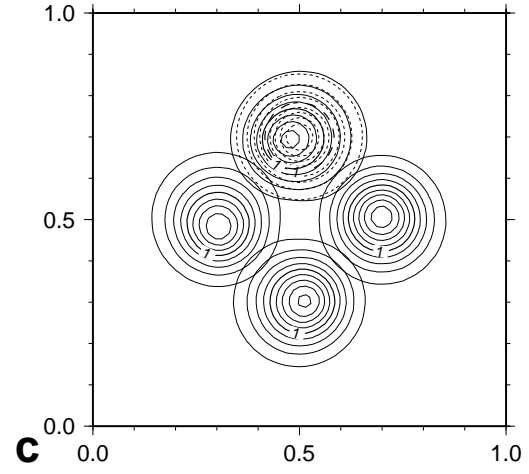
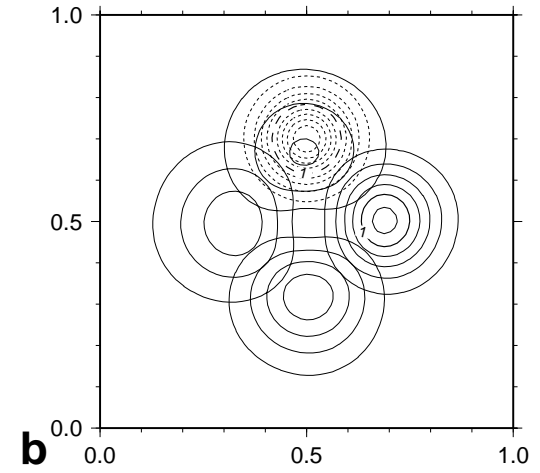
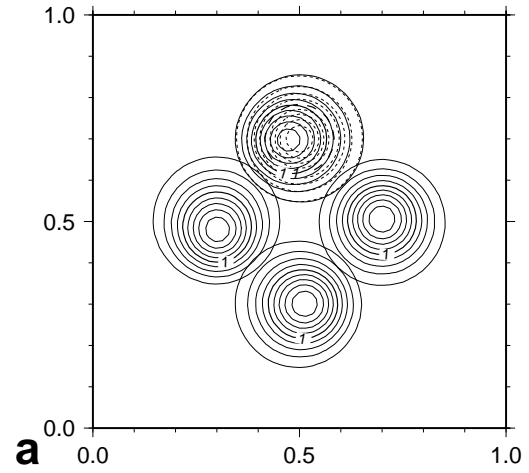


## Some useful 2-D advection fields

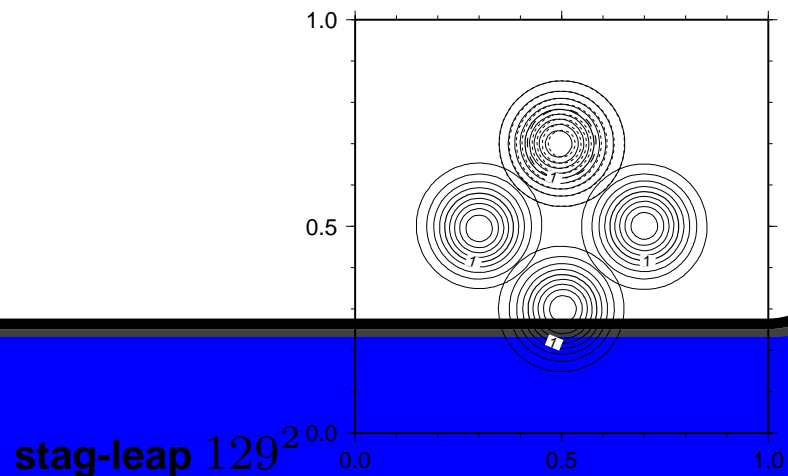
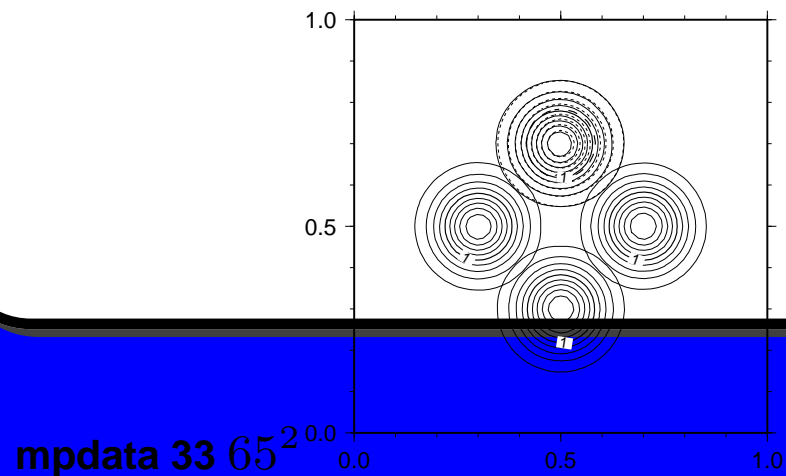
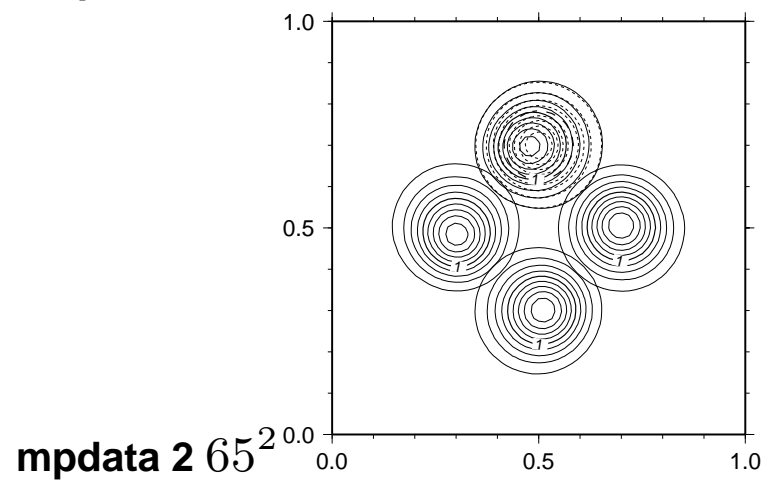
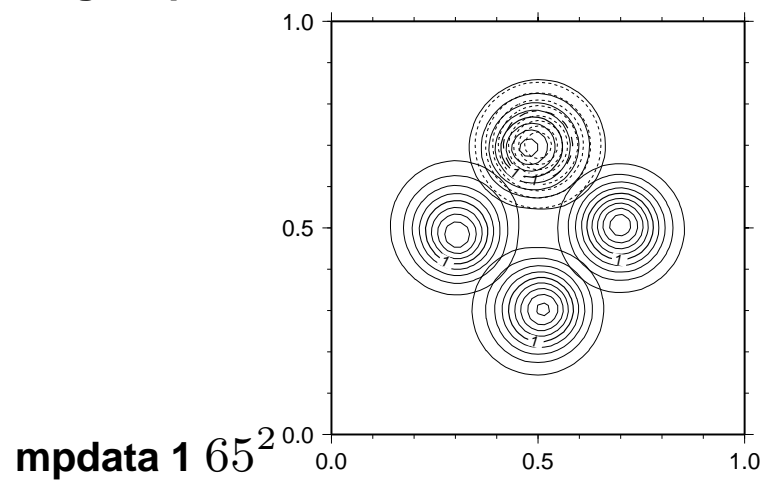
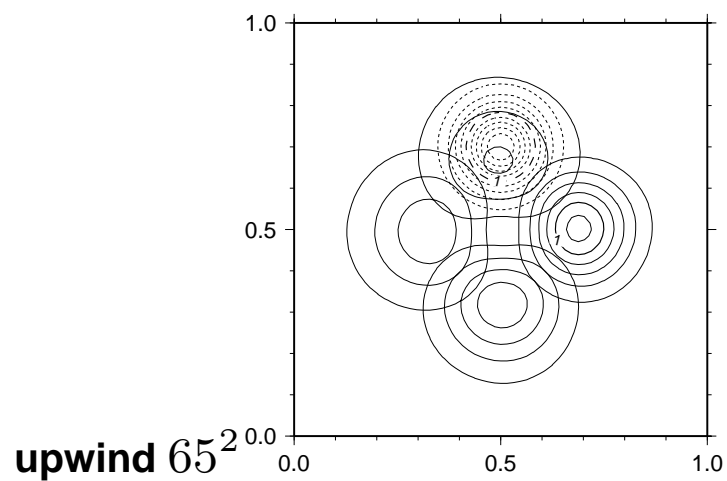
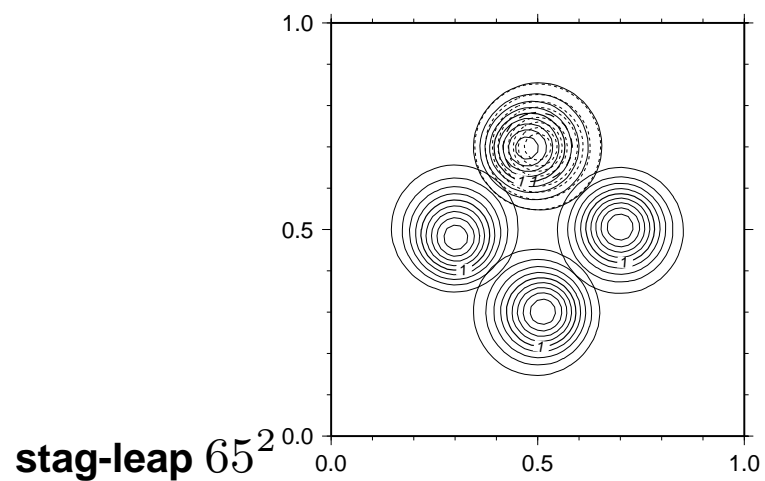
Rigid body rotation vs. a shear cell



**Rigid Body rotation test: a methods sampler**

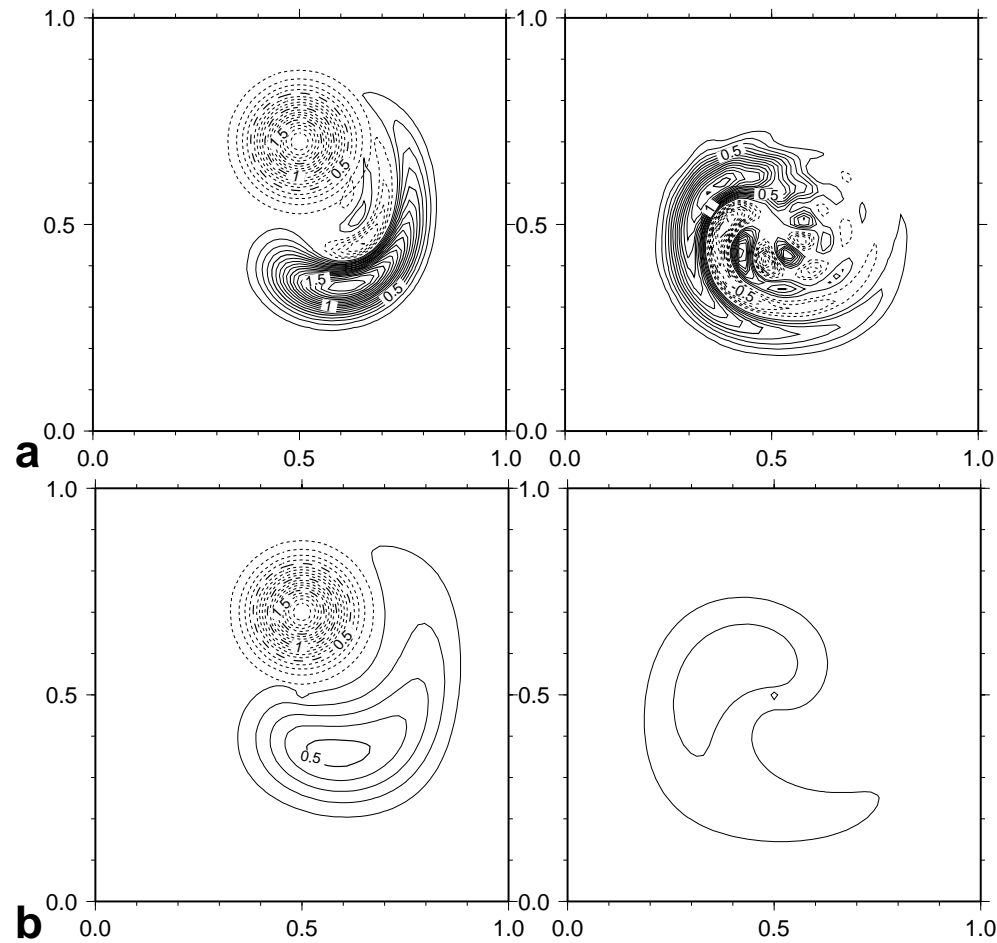


**Rigid Body rotation test: a methods sampler**



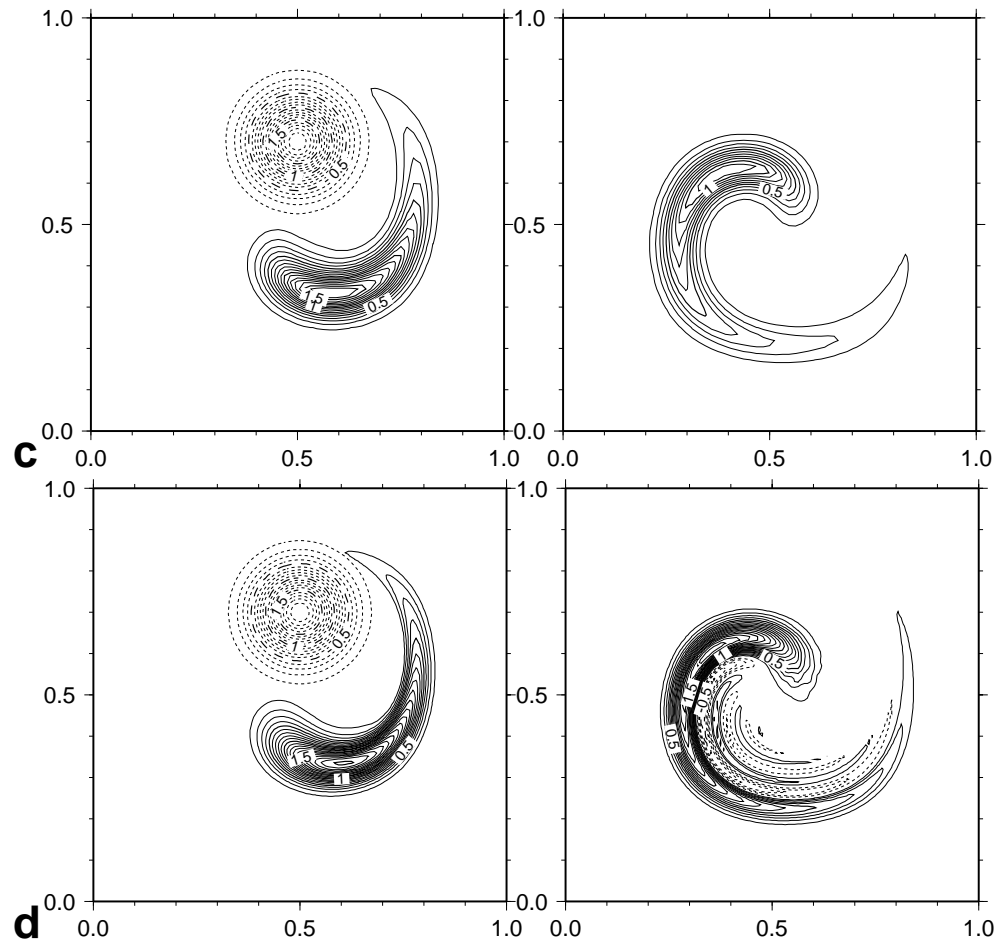
# Shear cell test

## Staggered Leapfrog vs. Upwind

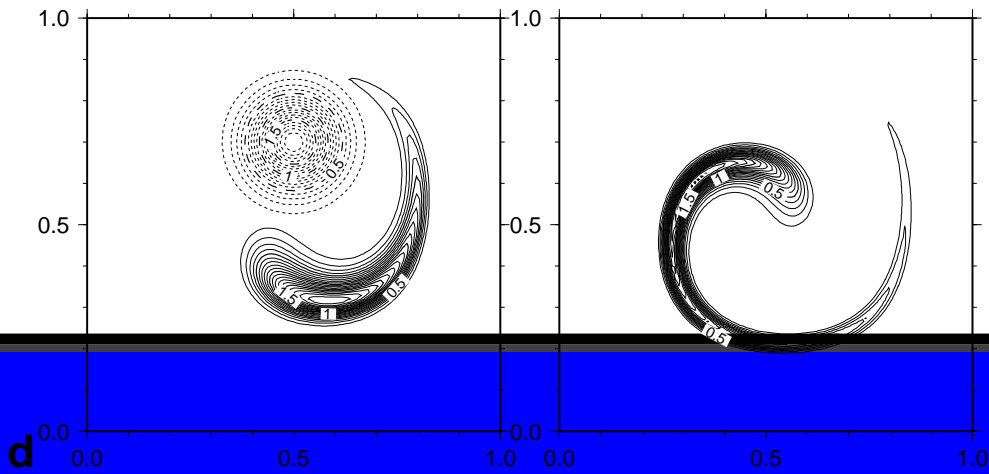
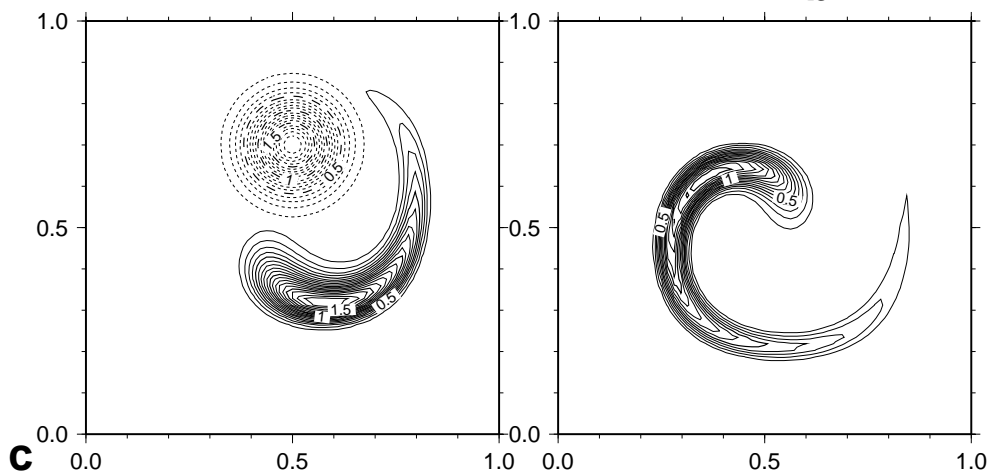
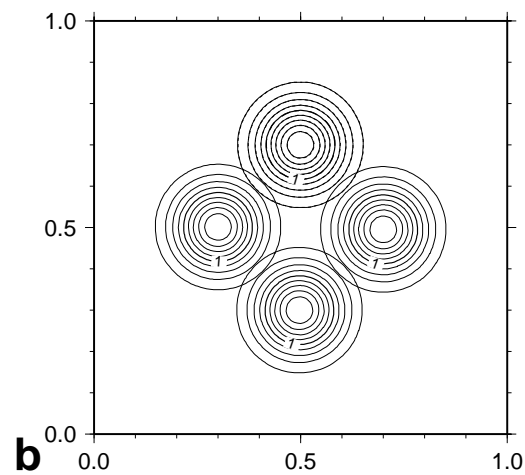
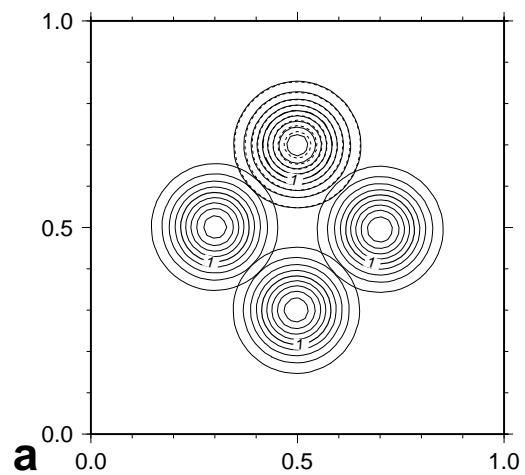


# Shear cell test

Mpdata (with everything) vs. High res Staggered Leapfrog

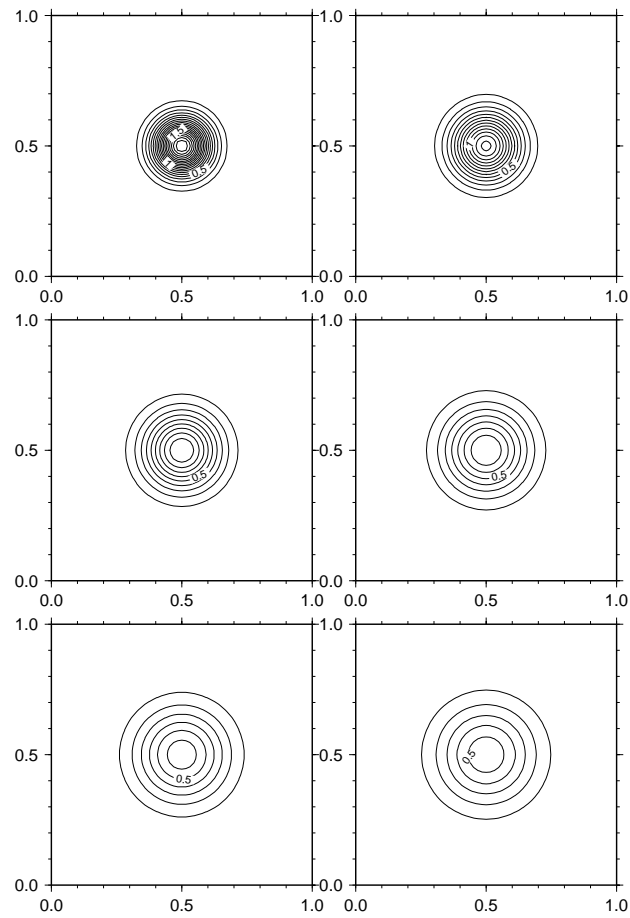


**The winner!**  
**Semi-Lagrangian behaviour**



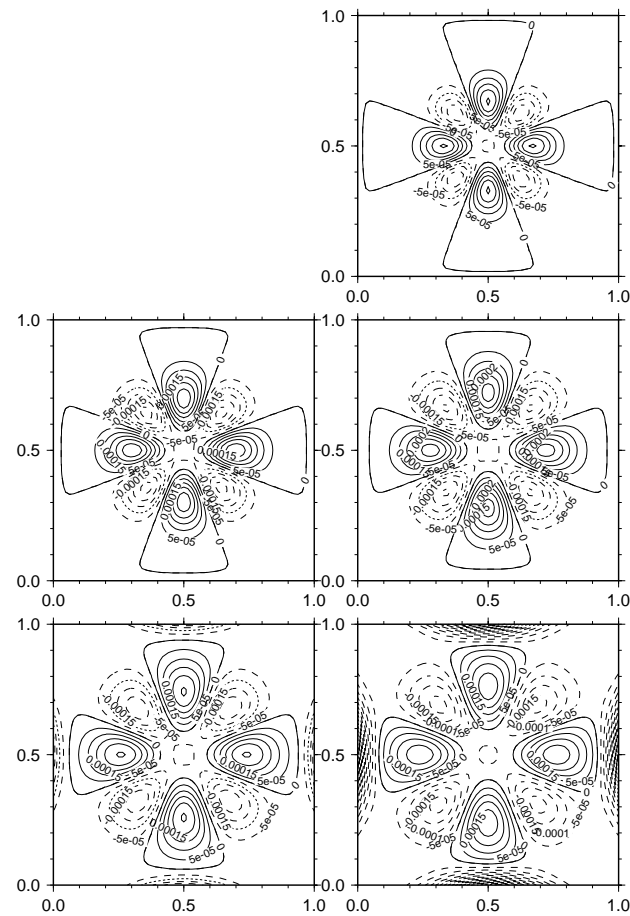
## 2-D Diffusion (booooring...)

### 2-D FTCS scheme



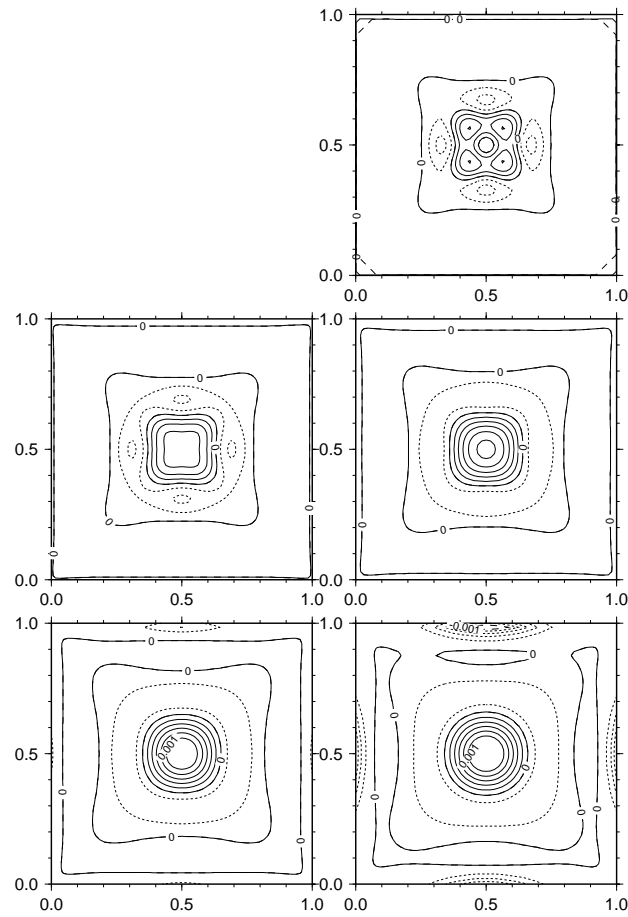
## 2-D Diffusion

### Errors for 2-D FTCS scheme

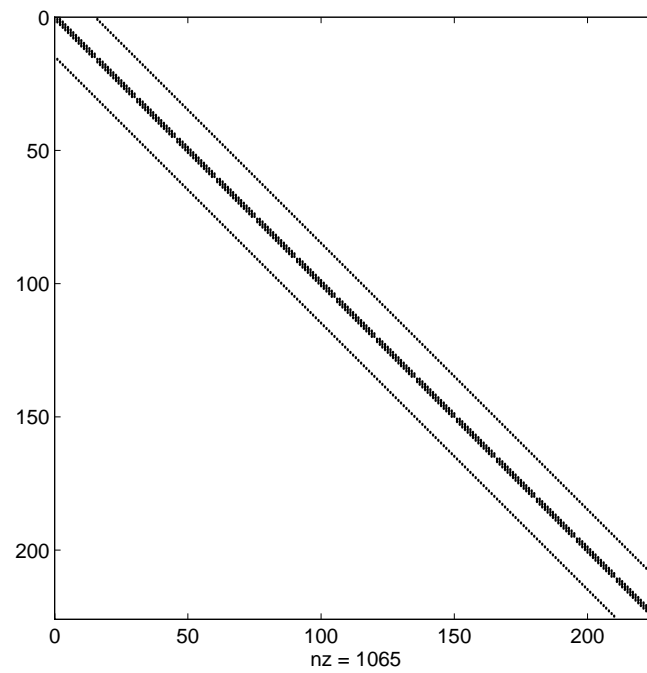


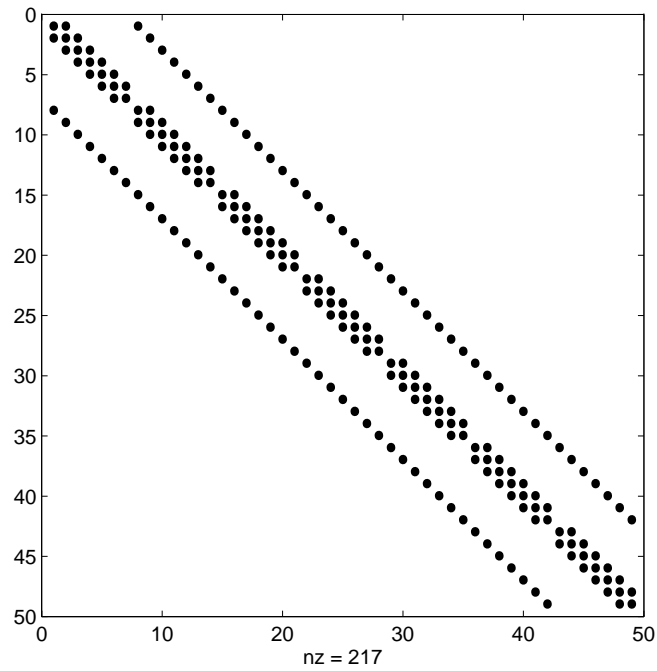
## 2-D Diffusion

### Errors for ADI scheme

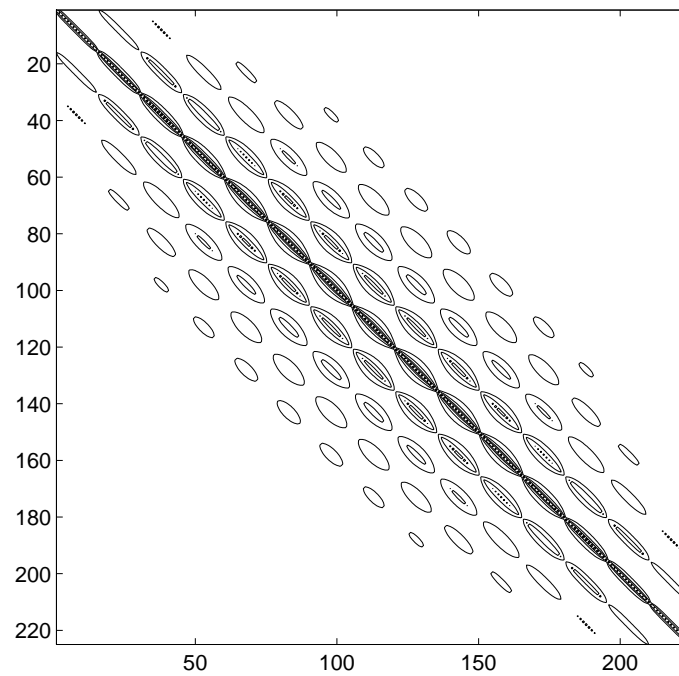


## Structure of the 5-point Laplacian Operator as a sparse matrix

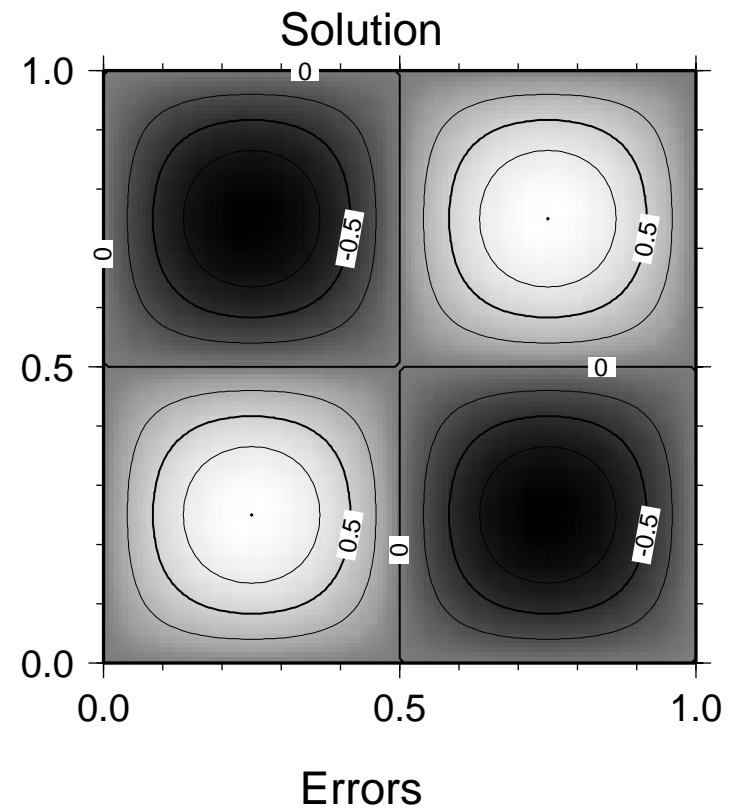


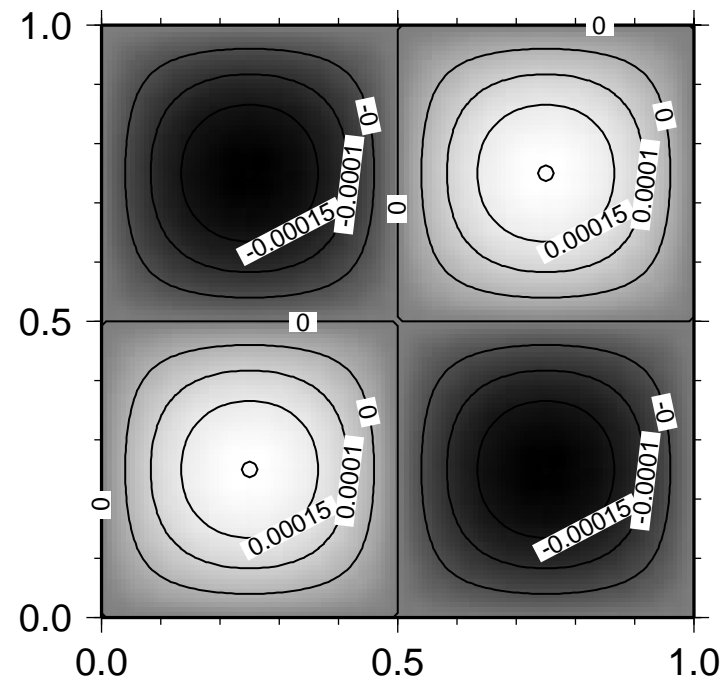


## Structure of the inverse of the 5-point Laplacian Operator as a sparse matrix

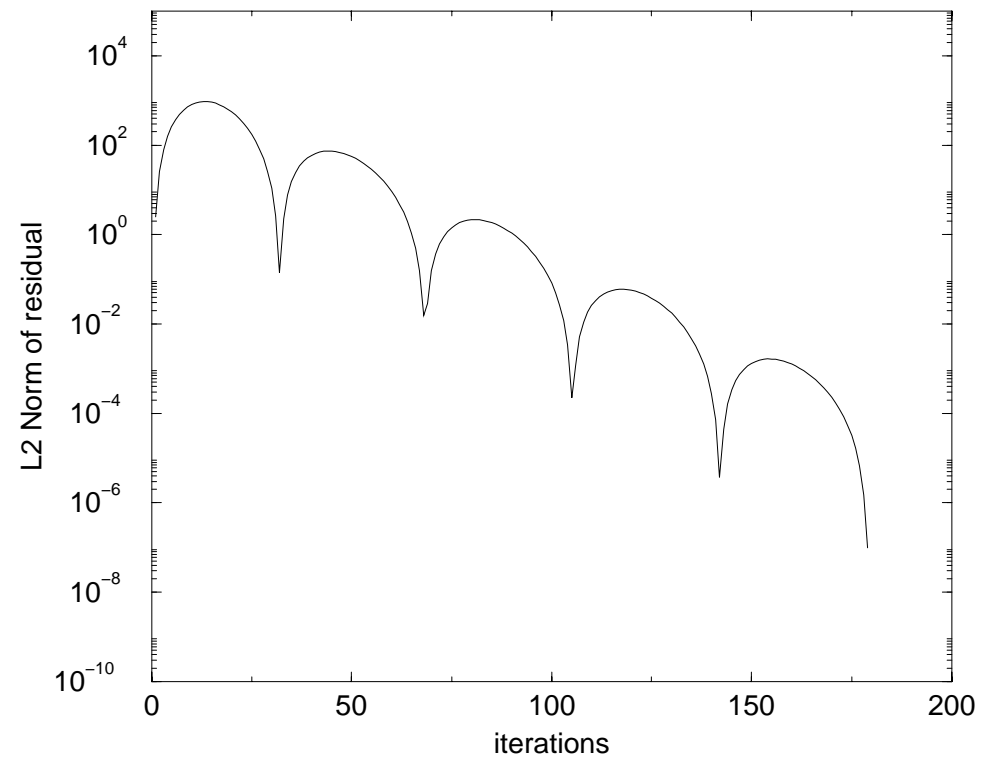


## Testing Laplace Solvers: the sin-cell test

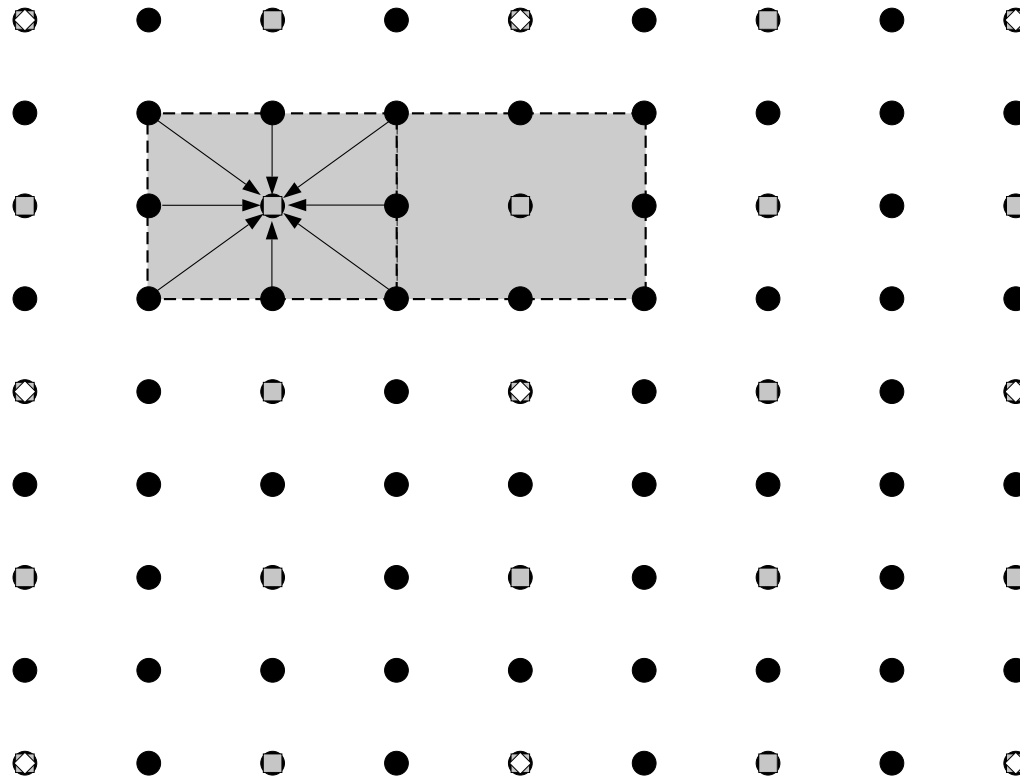




## Convergence Behaviour of optimal SOR

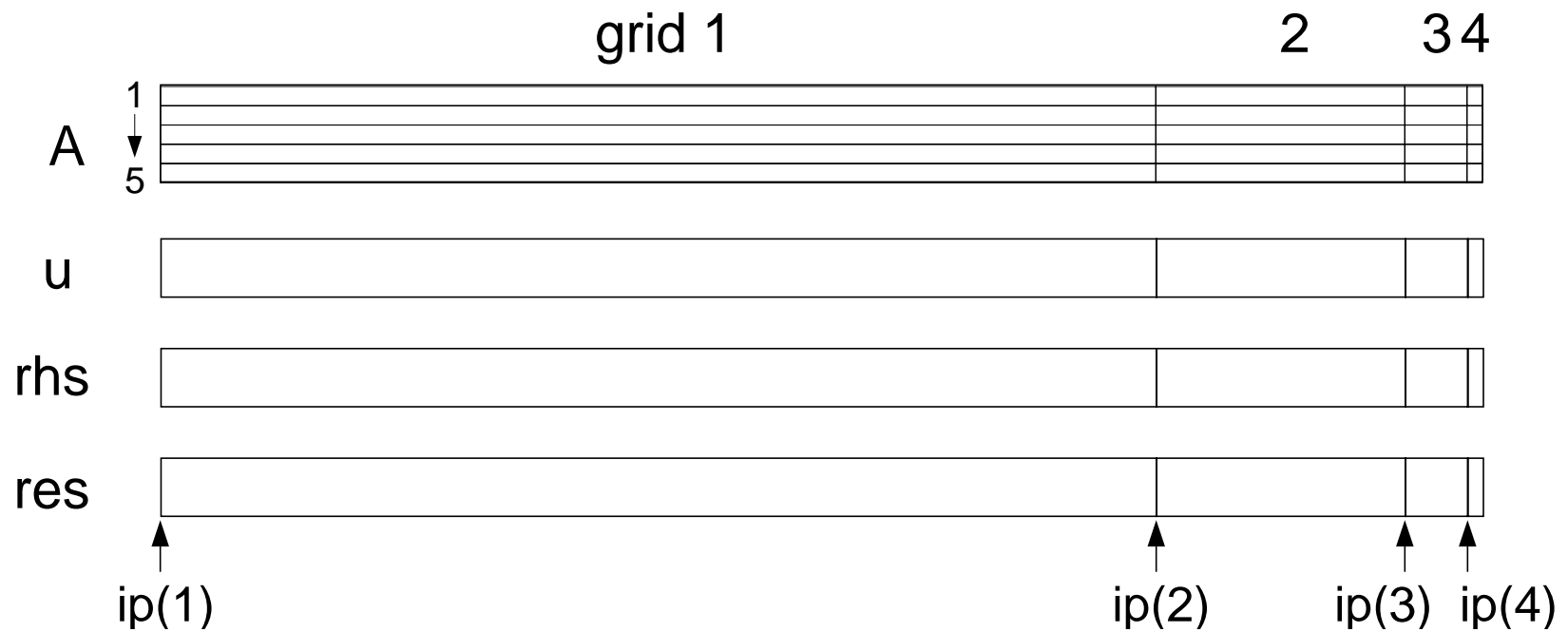


## A nested Multi-level Grid (A 3-level grid)

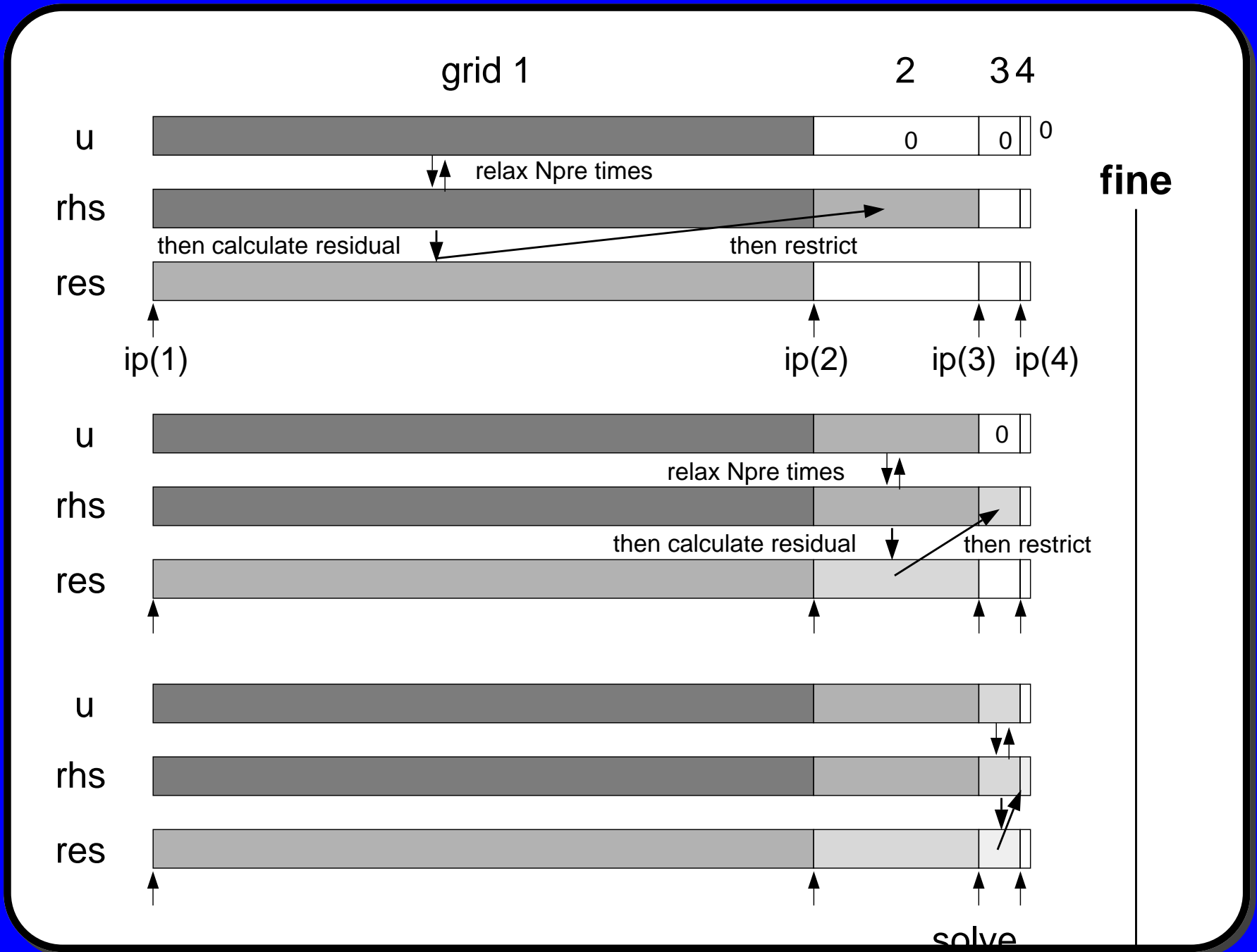




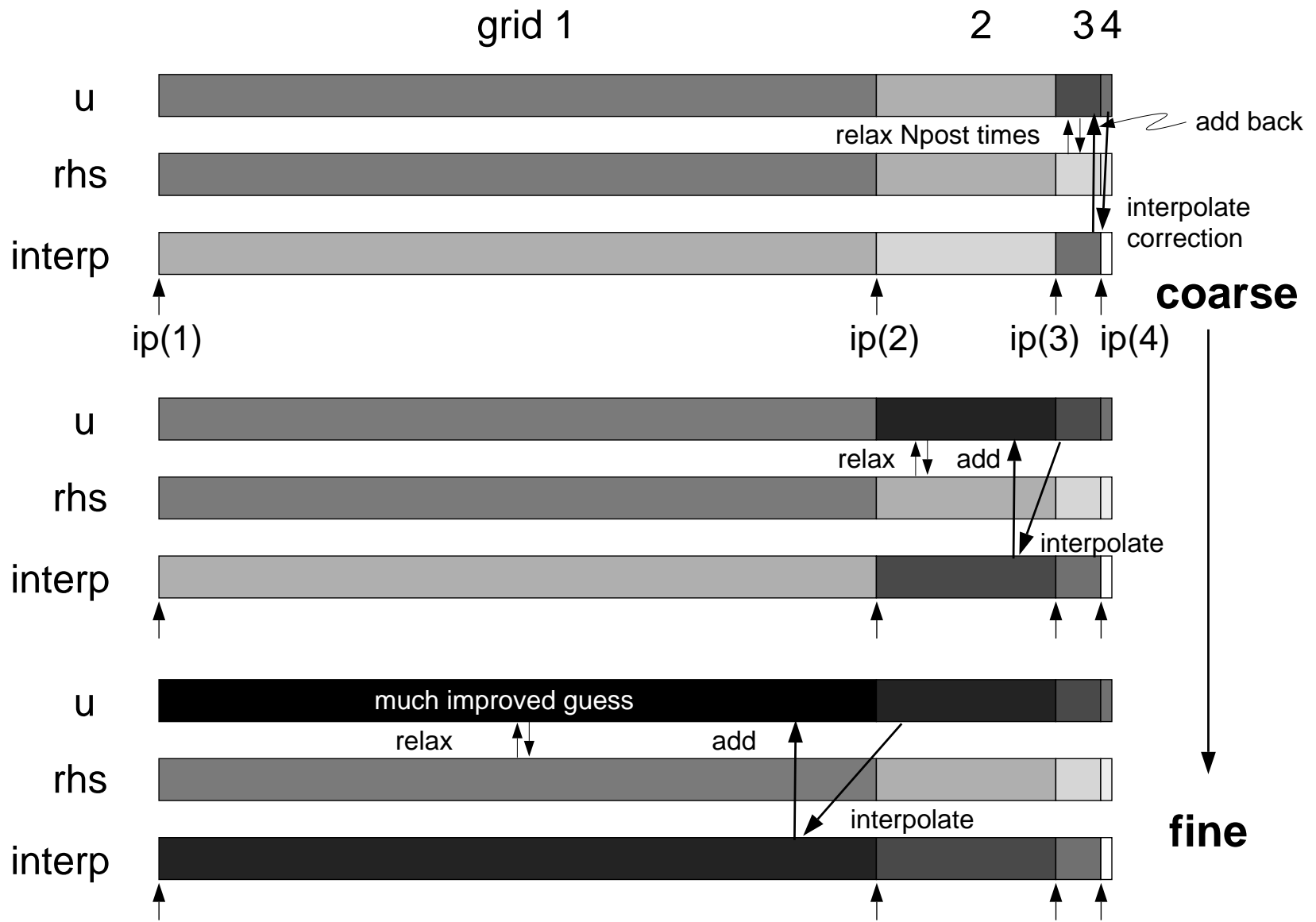
### Multi-Grid storage scheme ala Briggs



**A V-cycle in the Briggs Scheme**  
**Going up!**

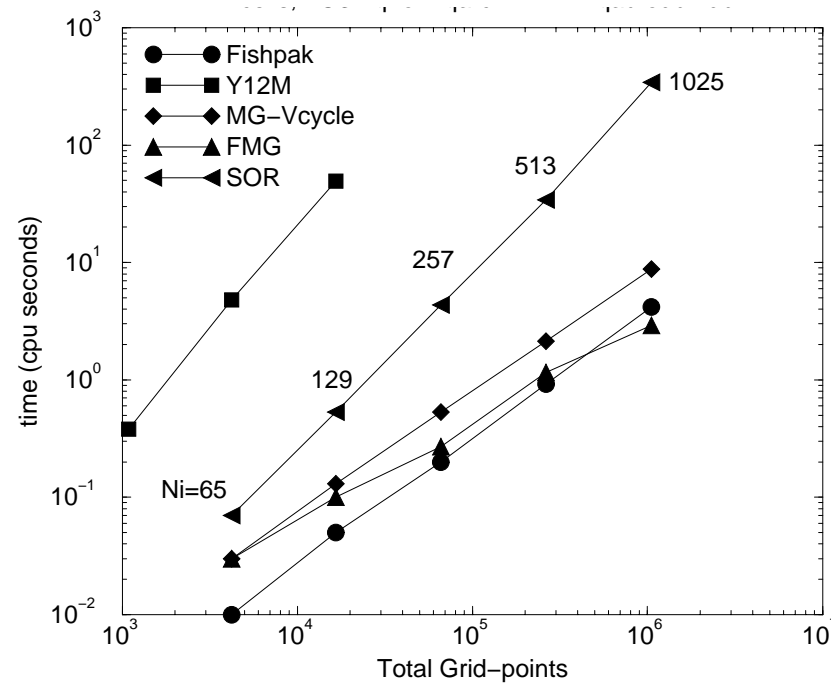


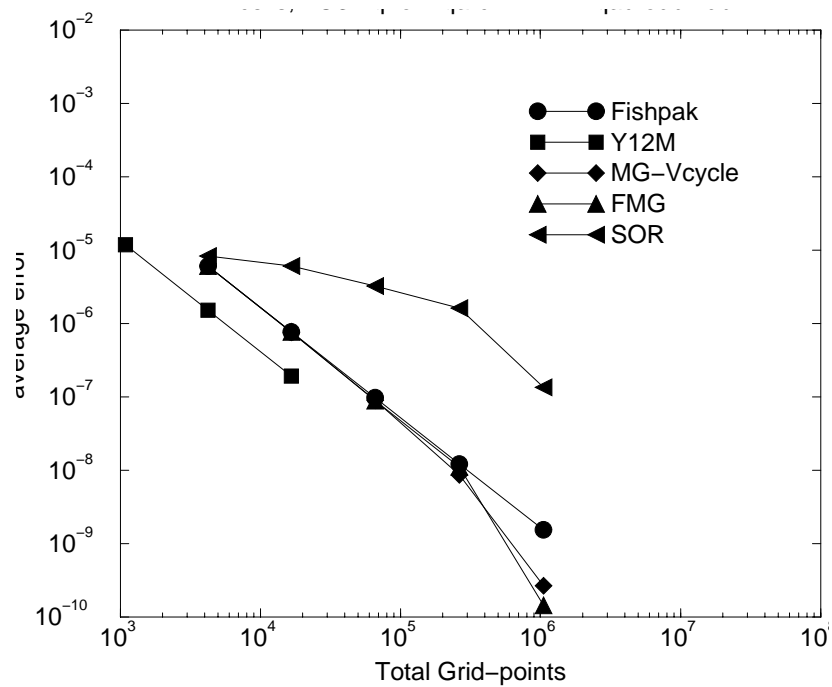
**A V-cycle in the Briggs Scheme  
Coming Down!**



## The Big test!

Timing and errors for solving Poisson problem with Dirichlet Boundaries on a 2-2 sin cell test





General Conservation of Mass for chemistry

$$\frac{\partial}{\partial t} \rho_s (1 - \phi) c^s + \nabla \cdot [\rho_s (1 - \phi) \mathbf{v} c^s] = -I + \mathcal{D}_s \quad (1)$$

$$\frac{\partial}{\partial t} \rho_f \phi c^f + \nabla \cdot [\rho_f \phi \mathbf{v} c^f] = I + \mathcal{D}_f \quad (2)$$

For Fractional melting  $I = (c^s / D) \Gamma$ , therefore

$$\frac{\partial}{\partial t} \rho_s (1 - \phi) c^s + \nabla \cdot [\rho_s (1 - \phi) \mathbf{v} c^s] = -\frac{c^s}{D} \Gamma \quad (3)$$

$$\frac{\partial}{\partial t} \rho_f \phi c^f + \nabla \cdot [\rho_f \phi \mathbf{v} c^f] = \frac{c^s}{D} \Gamma \quad (4)$$

Expanding By chain rule gives

$$c^s \left[ \frac{\partial}{\partial t} \rho_s (1 - \phi) + \nabla \cdot [\rho_s (1 - \phi) \mathbf{v}] \right] +$$

$$\rho_s (1 - \phi) \left[ \frac{\partial c^s}{\partial t} + \mathbf{v} \cdot \nabla c^s \right] = -\frac{c^s}{D} \Gamma$$

$$c^f \left[ \frac{\partial}{\partial t} \rho_f \phi + \nabla \cdot [\rho_f \phi \mathbf{v}] \right] +$$

$$\rho_f \phi \left[ \frac{\partial c^f}{\partial t} + \mathbf{v} \cdot \nabla c^f \right] = \frac{c^s}{D} \Gamma$$

But Conservation of total mass is

$$\frac{\partial}{\partial t} \rho_s (1 - \phi) + \nabla \cdot [\rho_s (1 - \phi) \mathbf{v}] = -\Gamma \quad (5)$$

$$\frac{\partial}{\partial t} \rho_f \phi + \nabla \cdot [\rho_f \phi \mathbf{v}] = \Gamma \quad (6)$$

Therefore we can write the problem as

$$-c^s\Gamma + \rho_s(1 - \phi)\frac{D_s c^s}{Dt} = -\frac{c^s}{D}\Gamma \quad (7)$$

$$c^f\Gamma + \rho_f\phi\frac{D_f c^f}{Dt} = \frac{c^s}{D}\Gamma \quad (8)$$

Rearranging

$$\frac{D_s c^s}{Dt} = -c^s \left( \frac{1}{D} - 1 \right) \frac{\Gamma}{\rho_s (1 - \phi)} \quad (9)$$

$$\frac{D_f c^f}{Dt} = \left( \frac{c^s}{D} - c^f \right) \frac{\Gamma}{\rho_f \phi} \quad (10)$$

and Scaling with

$$\phi = \phi_0 \phi'$$

$$t = \frac{w_0}{\delta} t'$$

$$\Gamma = \frac{\rho_s \phi_0 w_0}{\delta} \Gamma'$$

$$c^s = c_0^s c^{s'}$$

$$c^f = \frac{c_0^s}{D} c^{f'}$$

Yields

$$\frac{D_s c^s}{Dt} = -\frac{\phi_0}{(1 - \phi_0 \phi)} c^s \left( \frac{1}{D} - 1 \right) \Gamma \quad (11)$$

$$\frac{D_f c^f}{Dt} = (c^s - c^f) \frac{\rho_s \Gamma}{\rho_f \phi} \quad (12)$$

## Numerics

General Semi-Lagrangian solution of

$$\frac{Dc}{Dt} = g(c, \mathbf{x}, t)$$

is

$$\frac{c^+ - c^-}{\Delta t} = \frac{1}{2} [g^+ + g^-]$$

or

$$c^+ = c^- + \frac{\Delta t}{2} [g^+ + g^-]$$

Therefore for solid concentration can discretize

$$\frac{D_s c^s}{Dt} = -\frac{\phi_0}{(1 - \phi_0 \phi)} c^s \left( \frac{1}{D} - 1 \right) \Gamma$$

as

$$c^{s+} - c^{s(s-)} = -(Ac^s)^+ - (Ac^s)^{(s-)}$$

where

$$A = \frac{\Delta t \phi_0}{2(1 - \phi_0 \phi)} \left( \frac{1}{D} - 1 \right) \Gamma$$

therefore

Same for melt concentration;

$$\frac{D_f c^f}{Dt} = (c^s - c^f) \frac{\rho_s \Gamma}{\rho_f \phi} \quad (13)$$

Becomes

$$c^{f+} - c^{f(f-)} = [B(c^s - c^f)]^+ + [B(c^s - c^f)]^{(f-)}$$

where

$$B = \frac{\Delta t \rho_s \Gamma}{2 \rho_f \phi}$$

Therefore

$$(1 + B^+) c^{f+} = (1 - B^{(f-)}) c^{f(f-)} + (B c^s)^+ + (B c^s)^{(f-)}$$

or

$$c^{f+} = \frac{[(1 - B^{(f-)}) c^{f(f-)} + (B c^s)^+ + (B c^s)^{(f-)}]}{(1 + B^+)}$$

Final Update Scheme:

$$c^{s+} = \frac{(1 - A^{(s-)})}{(1 + A^+)} c^{s(s-)}$$

$$c^{f+} = \frac{\left[ (1 - B^{(f-)}) c^{f(f-)} + (Bc^s)^+ + (Bc^s)^{(f-)} \right]}{(1 + B^+)}$$