Preservation of Invariant Regions under Discretization

Donald J. Estep
Department of Mathematics
Colorado State University

Motivation: Detecting blow-up reliably using numerics

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Knowledge to Go Places

Blowup in Differential Equations

A solution or some of its derivatives become infinite at a finite time or at infinity

$$\begin{cases} u_t = u^2 \\ u(0) = 1 \end{cases} \quad \Rightarrow \quad u = \frac{1}{1-t}$$

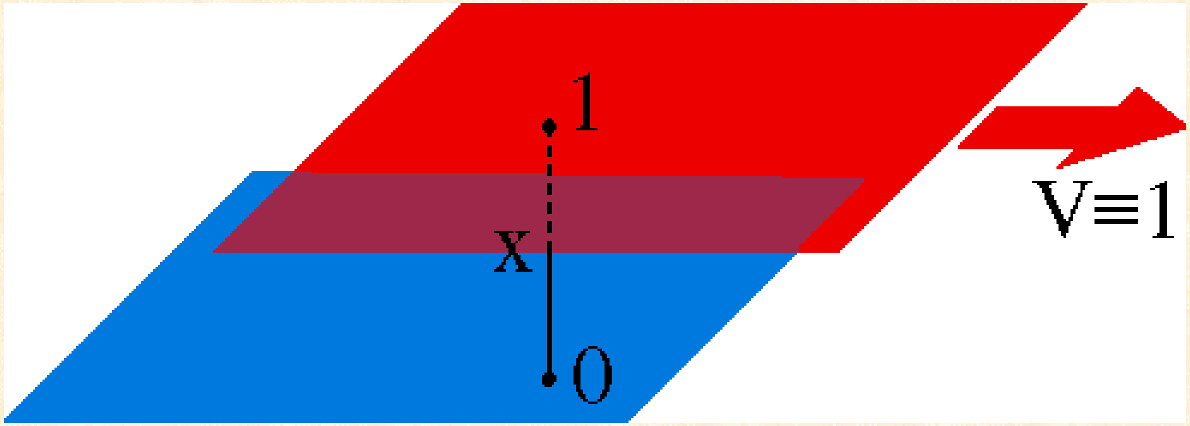
Numerical investigation is an important tool

Classic convergence analysis does not apply!

Can we trust numerical solutions?

- Can discretization prevent blow-up?
- Can discretization cause artificial blow-up?

Shear Flow with Temperature-Dependent Viscosity



θ = temperature, σ = shear stress, v = velocity

Assuming $\sigma = \theta^{-\alpha} v_x$, conservation of energy and momentum yields

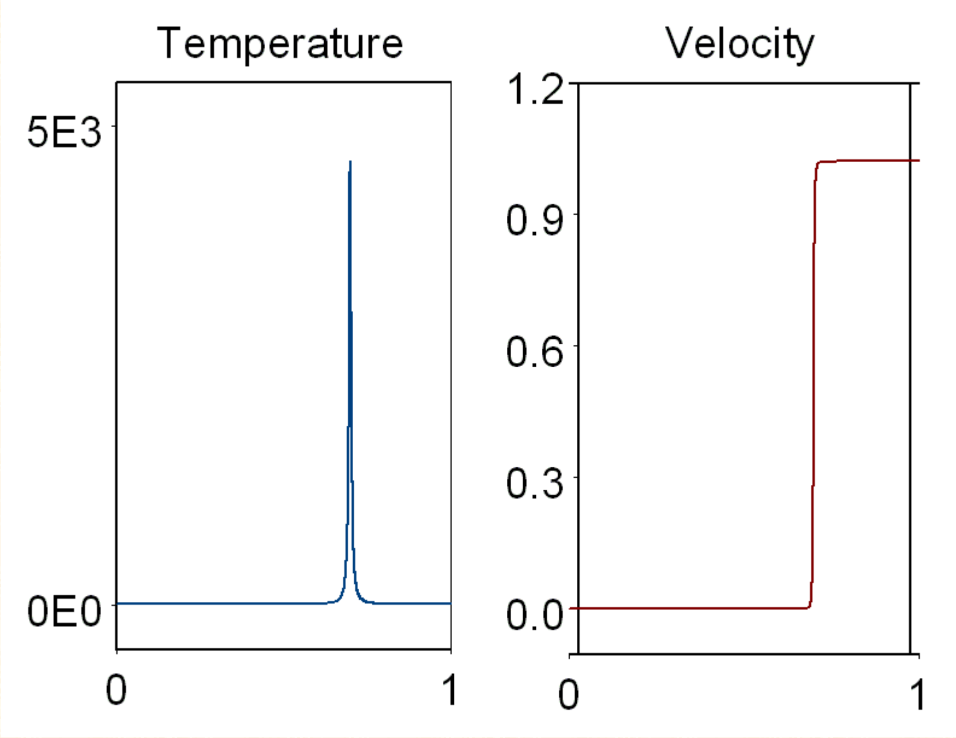
$$\begin{cases} \sigma_t - \theta^{-\alpha}\sigma_{xx} = -\alpha\theta^{\alpha-1}\sigma^3 \\ \theta' = \theta^{\alpha}\sigma^2 \end{cases}$$

Does Blow-up Occur?

Uniform shear flow: $v = x$

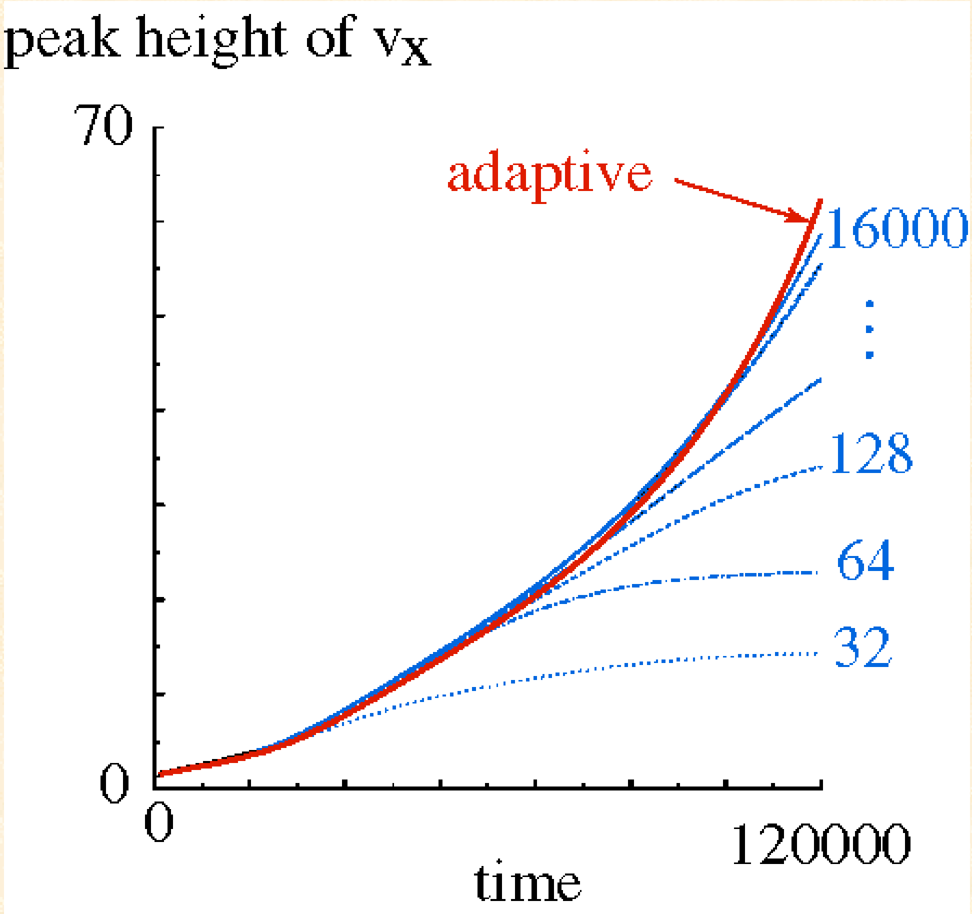
stable when $0 \le \alpha < 1$ unstable when $1 < \alpha$

Starting near the uniform shear flow with $\alpha = 2$,
here is the solution at $t \sim 17,0000$



Observing Blowup in the Shear Flow Model

Observations of blowup in numerical simulations depends critically on the accuracy of the numerical solutions



Blow-up in Reaction-Diffusion Equations

Can we trust numerical solutions?

- Can discretization prevent blow-up?

  Yes, inaccuracy can inhibit blow-up.
  We can use adaptive error control to maintain accuracy during the onset of blowup

- Can discretization cause artificial blow-up?

Invariant Regions

A set in solution space inside of which a solution remains for all time

A compact invariant region can imply global existence and smoothness of solutions

Example: $u_t = u^2$

u^2 is not globally Lipschitz continuous

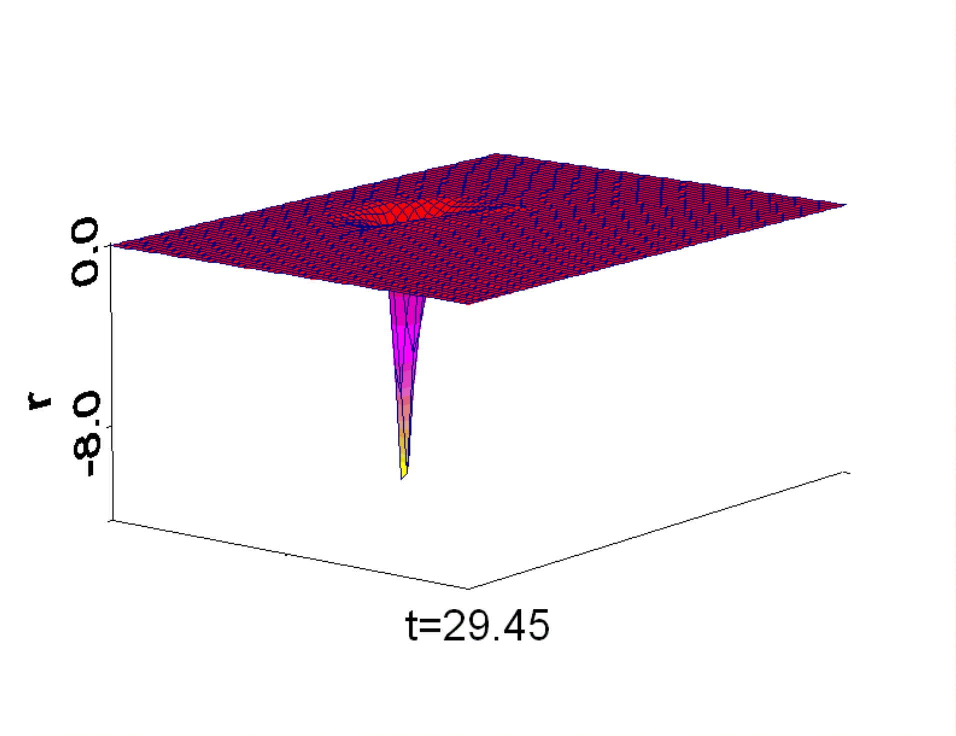
As u increases, so does the Lipschitz constant of u^2, driving the blowup

If a solution remains in a compact region, a local Lipschitz condition on the reaction serves as well as a global Lipschitz condition

SIR Model of Rabies in Foxes

$$\begin{cases} s_t = .003\left(1-(s+q+r)\right)s - rs \\ q_t = rs - \left(.08+.003+.003(s+q+r)\right)q \\ r_t - \Delta r = .08q - \left(.46+.003(s+q+r)\right)r \end{cases} \Rightarrow r > 0 \text{ is invariant}$$

A numerical solution from PDEASE®



Blow-up in Reaction-Diffusion Equations

Can we trust numerical solutions?

- Can discretization prevent blow-up?
- Can discretization cause artificial blow-up?

Yes, numerical solutions can exhibit spurious blow-up. We can use schemes that automatically preserve invariant regions

If blowup is seen in a numerical solution that preserves compact invariant regions, this is strong evidence that blowup is occurring

Simplified Problem

$u = (u_i) \in \mathbb{R}^D$ solves

$$(u_i)_t - \varepsilon_i \Delta u_i = f_i(u), \quad x \in \Omega,\ t > t_0$$

where

$$\varepsilon_i > 0, \quad 1 \le i \le d$$

$$\varepsilon_i = 0, \quad d < i \le D$$

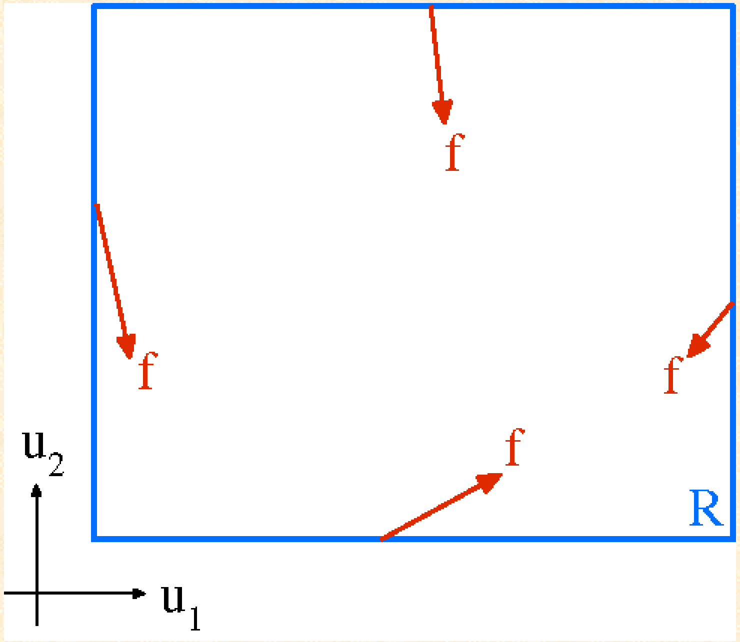
Invariant Rectangle

A generalized rectangle in solution space with sides parallel to the coordinate planes

Invariant rectangle condition on R

$$n_{\partial R}(u) \cdot f(u, \cdot, \cdot) \leq 0 \quad u \in \partial R$$

$n_{\partial R}(u)$ is the outward unit normal to ∂R



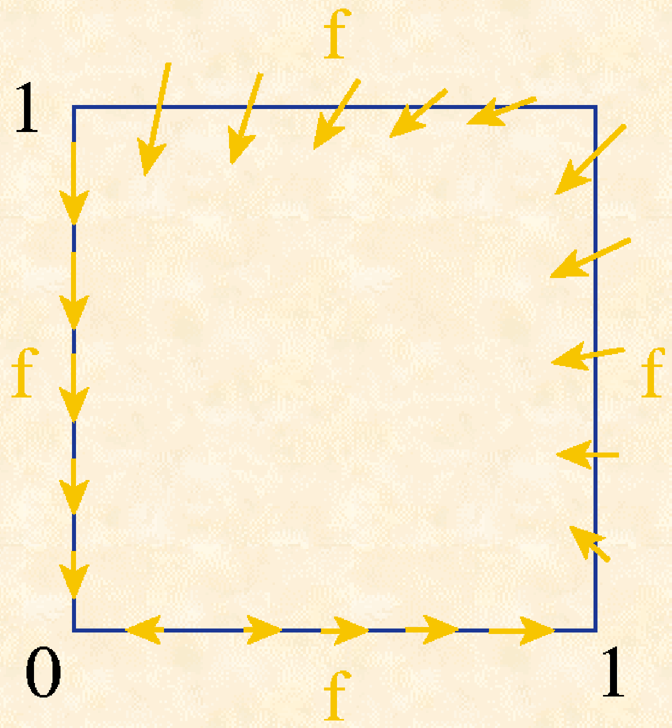
Invariant Rectangle

Essentially, two facts give invariance

- $u_t - \varepsilon \Delta u$ satisfies a maximum principle
- The sign of f on the boundary means that it pushes solutions near the boundary back inside the rectangle

Predator-Prey Model

$$\begin{cases} (u_1)_t - .01\Delta u_1 = -u_1\left((u_1 - .25)(u_1 - 1) + 2u_2\right) \\ (u_2)_t - .01\Delta u_2 = -u_2\left(1 + 3.4u_2 - 2u_1\right) \end{cases}$$



Interesting dynamics can occur inside the rectangle!

Applications with Invariant Rectangles

Allen-Cahn equation

predator-prey model

Hodgkin-Huxley equations

Fitz-Hugh-Nagumo equations

superconductivity in liquids

Field-Noyes equations

flame propagation

models for morphogenesis

model of rabies in foxes in Europe

Can We Preserve Invariant Rectangles?

- Preservation of exact invariant rectangles
- Preservation of approximate invariant rectangles

Exact Preservation

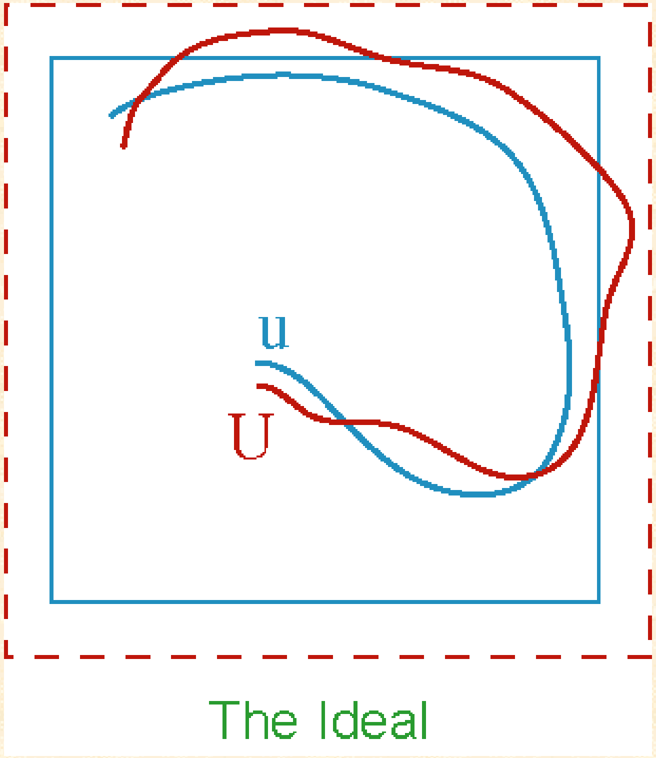
This is related to whether the numerical method satisfies a maximum principle when applied to the heat equation

For the standard finite element method, this requires the use of the lumped mass quadrature formula for the space integrals

Under a severe CFL-like stability restraint on the time steps, any invariant rectangle for the true solution is also invariant for the lumped mass finite element solution

Preserving Approximate Invariant Rectangles

We try to keep the numerical solution inside an approximation of the invariant rectangle by using adaptive error control



But error bounds grow exponentially with time!

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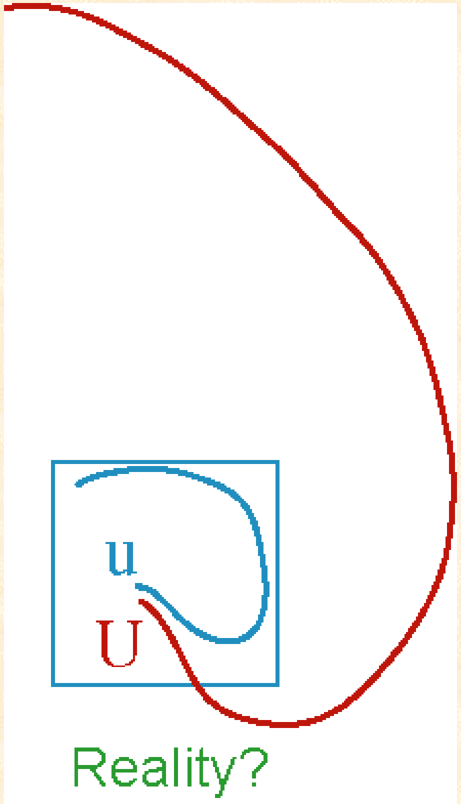
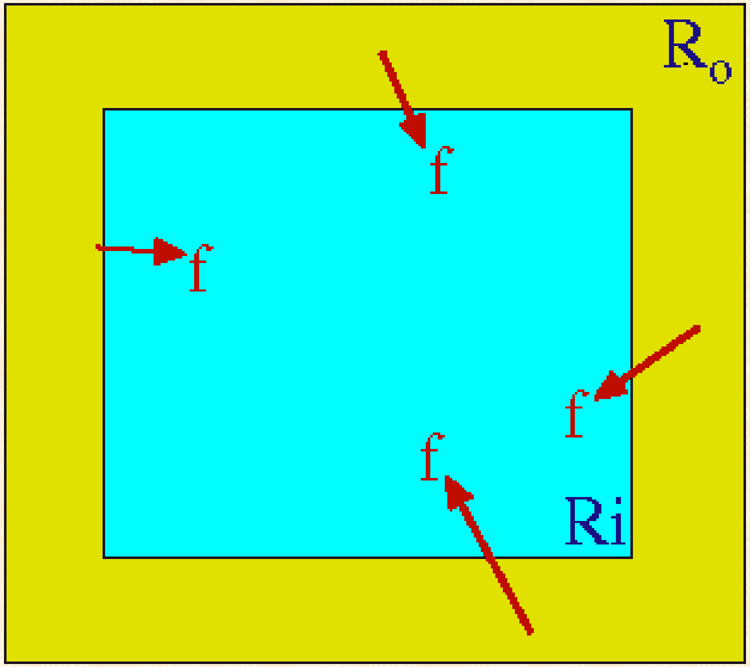


But error bounds grow exponentially with time!

Preservation of a "Fuzzy" Rectangle

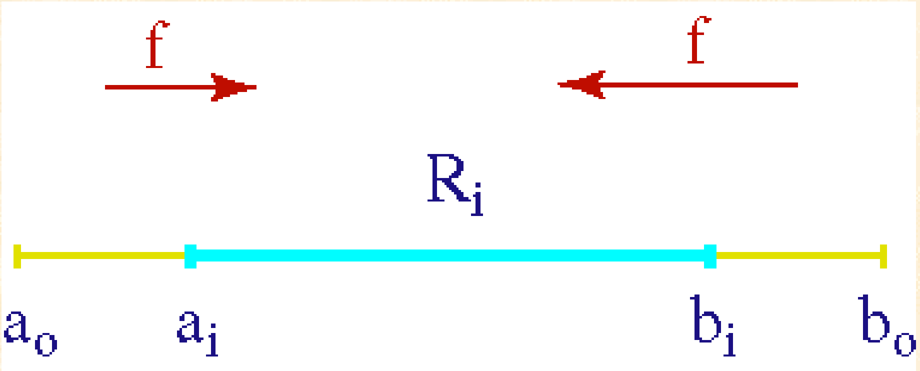
We assume there are concentric rectangles $R_i \subset R_o$ such that f satisfies a minimum angle condition in the region between R_i and R_o



A solution starting with data in the outer rectangle R_o must enter the inner rectangle R_i after a fixed finite time

Ordinary Differential Equations

$$\begin{cases} u_t = f(u) \\ u(t_0) = u_0 \end{cases}$$



$$u > b_i \text{ and } u_t = f(u) \le -M$$

$$\Rightarrow u(t) - b_i \le u_o - b_i - M(t - t_0)$$

$$u \text{ enters } R_i \text{ after } t^* = t_0 + \frac{b_0 - b_i}{M}$$

Reaction-Diffusion Equations

It is more complicated for reaction-diffusion equations because a solution can increase and decrease simultaneously

We perform the analysis on the Lipschitz continuous functional defined by the size of the smallest rectangle concentric with R_i containing the solution

Controlling the Accuracy

We control the accuracy using an *a posteriori* error estimate

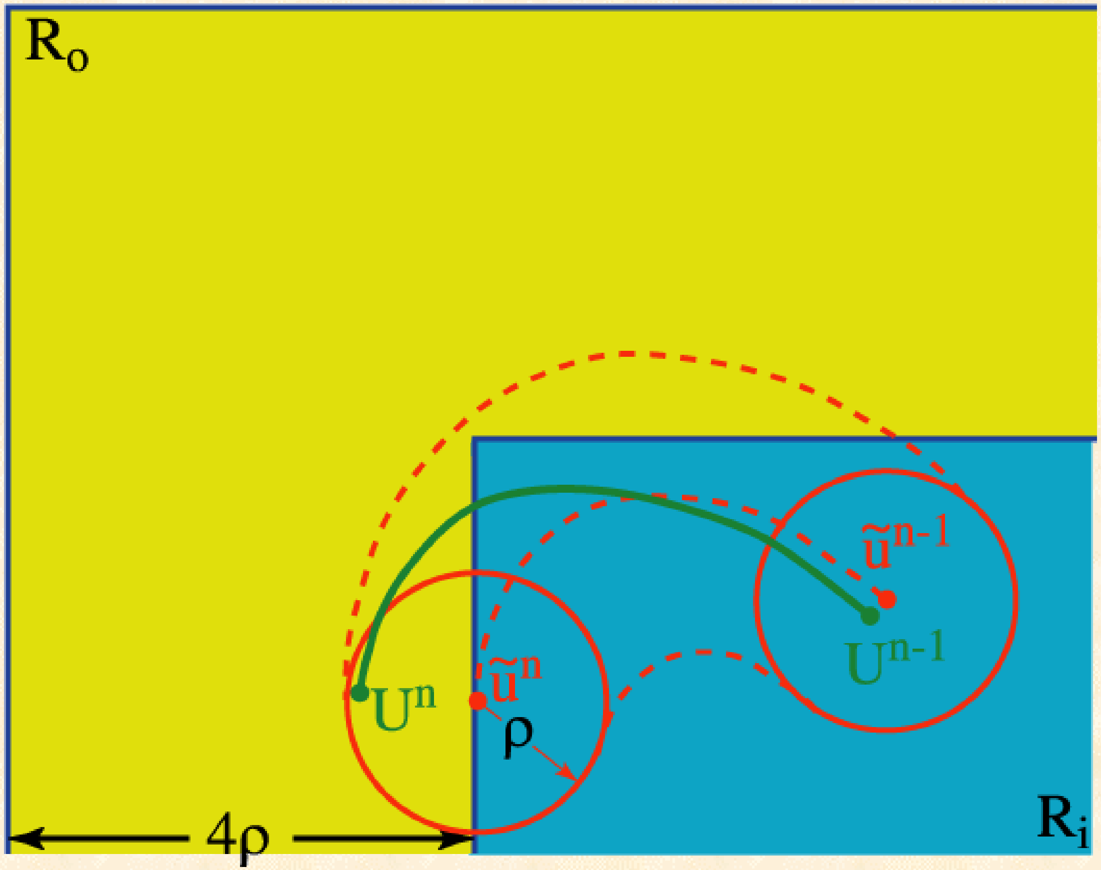
$$\left\|e(t)\right\| \le e^{C(t-t_0)}\left(\max_{t_o \le s \le t} \mathbf{R}(U(s)) + \left\|e(t_0)\right\|\right)$$

$$\mathbf{R}(U)\big|_i \;\text{"="}\; \left\|\left((U_i)_t - \varepsilon_i \Delta U_i - f_i(U)\right)\left(h^2 + k\right)\right\|$$

The residual can always be made small by refinement

Case 1

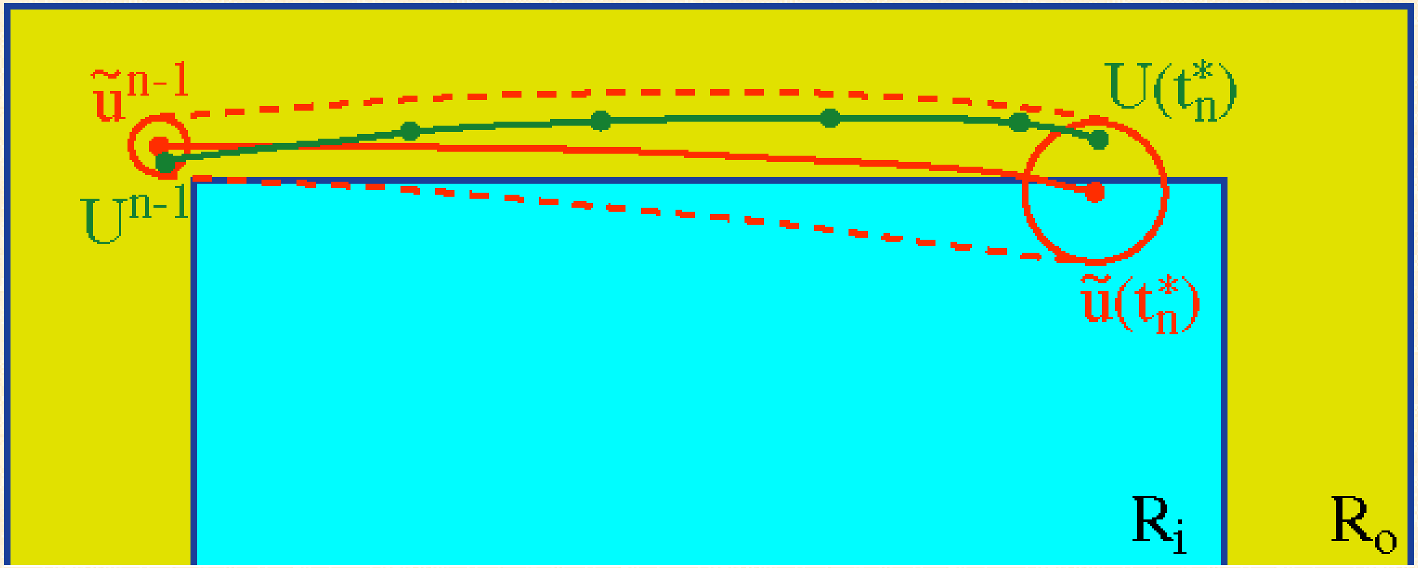
U^{n-1} is inside R_i



We compare U to a nearby "local" solution

Case 2

U^{n-1} is inside $2\rho + R_i$ and outside R_i



Theorem on Approximate Preservation

If the residual is kept smaller than a tolerance that depends on the

- width of the fuzzy region $R_o \setminus R_i$
- angle in the minimum angle condition
- size and shape of R_i
- Lipschitz constant and size of f in R_o

but is independent of time then U remains inside a small multiple of R_i for all time

References

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