Taming explosive computational instability: Compensated explicit time-marching schemes in multidimensional, nonlinear, well-posed or ill-posed initial value problems for partial differential equations

Alfred S. Carasso
Applied and Computational Mathematics Division
NIST, Gaithersburg, Maryland.

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Consider well-posed forward problem $w_t = Lw,\ t > 0$, with L a 2nd order elliptic differential operator.

Pure Explicit $w^{n+1} = w^n + \Delta t L w^n$, **ideal.**

Leapfrog $w^{n+1} = w^{n-1} + 2\Delta t L w^n$, **better.**

Crank-Nicholson $2w^{n+1} + \Delta t L w^{n+1} = 2w^n + \Delta t L w^n$.

Pure Explicit $\Rightarrow$ **impractically small** Δt (Courant).

Leapfrog **always unstable** no matter how small Δt.

Crank-Nicholson $\Rightarrow$ **large** algebraic problem at each n.

Stabilize explicit schemes. Apply to difficult multidimensional nonlinear well-posed forward problems. Avoid **implicit** scheme algebraic computations at each n.

Stabilized schemes can also be run **backward** in time. Solve previously **intractable** ill-posed problems.

EXAMPLES OF IRREVERSIBLE PDE PROBLEMS

Advection dispersion equation
$w_t = \sigma \Delta w - \nabla.(\beta \ w)$

Wave propagation in viscous fluid
$w_{tt} = c^2 \Delta w + \gamma \Delta w_t$

Coupled sound and heat flow
$w_{tt} = c^2 \Delta w - c^2 \Delta u,$
$u_t = \sigma \Delta u - \lambda w_t$

Nonlinear variations. Other coupled systems.

ENVIRONMENTAL FORENSICS
Groundwater Pollution

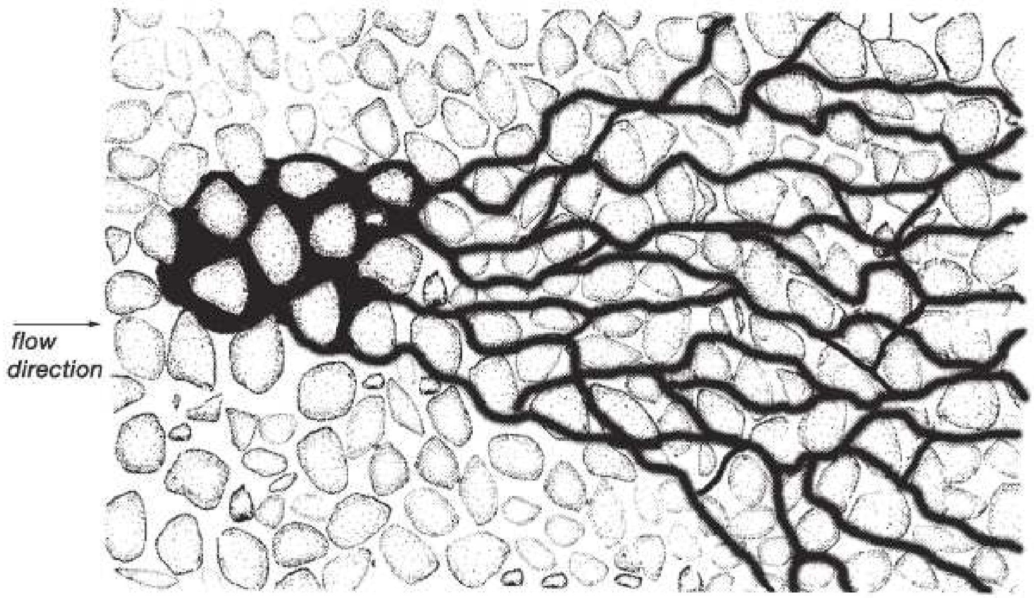
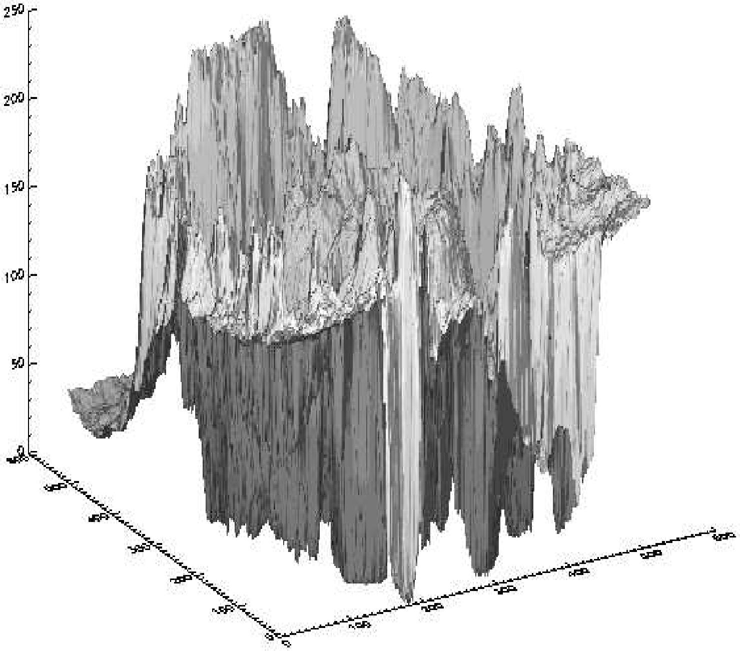


Fig. 1 Contaminant transported in porous media

Identify source of groundwater contamination by solving advection dispersion eqn backward in time.

IMAGES MAKE GOOD TEST PROBLEMS

Shirley Temple image **Plot of intensity values**



Consider PDE problem: $w_t = Lu,\ 0 \le t \le T,\ \ w(0) = f.$

Assume L **linear** selfadjoint second order elliptic operator, with variable coefficients independent of t.

Eigenvalues $\{\lambda_m\}_{m=1}^{\infty}; \quad 0 < |\lambda_1| \le |\lambda_2| \le \cdots \le |\lambda_m| \le\uparrow \infty$

PDE well-posed if all $\lambda_m < 0$, **ill-posed** if all $\lambda_m > 0$.

For any $q > 0$, operator $(L^2)^{q/2}$ has eigenvalues $|\lambda_m|^q$.

For small $\omega > 0,\ q \ge 2$, define **smoothing operator** $S = \exp\{-\omega \Delta t (L^2)^{q/2}\}$. **Define** $\beta_q = \omega^{1/(1-q)}$.

Operator S can be synthesized in terms of eigenpairs $\{\lambda_m,\ \phi_m\}$ of L, **assumed known or precomputed**.

Consider **compensated pure explicit scheme**
$w^{n+1} = Sw^n + \Delta t S L w^n, \quad n \ge 0, \quad w^0 = f.$

$S = \text{exp}\{-\omega \Delta t (L^2)^{q/2}\}, \quad \beta_q = \omega^{1/(1-q)},$

$w^{n+1} = Sw^n + \Delta t S L w^n, \quad n \geq 0, \quad w^0 = f.$

Theorem 1: Compensated pure explicit scheme **always stable** and $\| w^{n+1} \|_2 \leq (1 + \beta_q \Delta t) \| w^n \|_2$, if $n \geq 0$. Hence, if $t_n = n\Delta t$, $\| w(t_n) \|_2 \leq \text{exp}(\beta_q t_n) \| f \|_2$.

Leapfrog scheme $w^{n+1} = w^{n-1} + 2\Delta t L w^n, \quad n \geq 1.$
Put $v^n = w^{n-1}$, and consider equivalent system
$v^{n+1} = w^n, \quad w^{n+1} = v^n + 2\Delta t L w^n, \quad n \geq 1.$

Define $U^n = [v^n, w^n], \quad \| U^n \|_2^2 \equiv \| v^n \|_2^2 + \| w^n \|_2^2$

With ω, q, β_q, S, as above, **compensated leapfrog**,
$v^{n+1} = Sw^n, \quad w^{n+1} = Sv^n + 2\Delta t S L w^n, \quad n \geq 1.$

Theorem 2: Compensated leapfrog scheme **always stable**, and $\| U^{n+1} \|_2 \leq (1 + 2\beta_q \Delta t) \| U^n \|_2$, if $n \geq 1$. Hence, if $t_n = n\Delta t$, $\| U(t_n) \|_2 \leq \text{exp}(2\beta_q t_n) \| U(t_1) \|_2$.

Remark. Theorems valid even if $w_t = Lw$ **ill-posed !!!**

Replace inconvenient smoothing operator S with

Laplacian-based $\qquad S_{\triangle} = \exp\{-\epsilon\Delta t(-\Delta)^p\}$.

Known characteristic pairs of Δ in several geometries.

Rectangular domain $\Rightarrow$ fast FFT synthesis of $S_{\triangle}$.

Major Assumption: $\| S_{\triangle} g \|_2 \leq \| Sg \|_2$. More precisely, given $\omega > 0$, and $q > 2$, $\exists\ \epsilon > 0$ and real $p \geq q$, $\ni\ \forall g \in L^2$ and sufficiently small $\Delta t > 0$,

$$\| \exp\{-\epsilon\Delta t(-\Delta)^p\} g \|_2 \leq \| \exp\{-\omega\Delta t(L^2)^{q/2}\} g \|_2 .$$

Above inequality **not proved**. Appears verified in many interesting computational examples. Related to **Gaussian lower bounds for heat kernels**. Deep theory.

Theorems 1 and 2 remain valid with $S_{\triangle}$ replacing S.

Error bounds for well-posed $w_t = Lw,\ 0 \le t \le T$.

Given **exact** initial data f. Schemes **stable**, but do not **converge** as $\Delta t \downarrow 0$. Smoothing $\Rightarrow$ **residual error**.

Let $w_{ex}(t)$ be exact solution of $w_t = Lw, \quad 0 \le t \le T$.

Let $e(t_n) = w_{ex}(t) - w(t_n)$ be the error at $t_n = n\Delta t$.

Let $B = \sup_{0 \le t \le T} \ \{\| \ (-\Delta)^p w_{ex}(t) \ \|_2\}$.

For **compensated pure explicit well-posed** case

$\| \ e(t_n) \ \|_2 \le (B\epsilon/\omega)(e^{\beta_q t_n} - 1)/(\beta_q)^q + O(\Delta t)$

$(B\epsilon/\omega)(e^{\beta_q t_n} - 1)/(\beta_q)^q \equiv$ **Stabilization Penalty**.
Involves parameters $\epsilon,\ p,\ \omega,\ q$

For **compensated leapfrog well-posed** case

$\| \ e(t_n) \ \|_2 \le (B\epsilon/\omega)(e^{2\beta_q t_n} - 1)/2(\beta_q)^q + O(\Delta t^2)$

(larger stabilization penalty).

$(B\epsilon/\omega)(e^{\beta_q t_n}-1)/(\beta_q)^q \equiv$ **Explicit stabilization penalty**.

Example 1 If $\omega = 1.0E-8,\ q = 2.75,\ T = 1.0E-4,$
then $\beta_q = 37276,\ (e^{\beta_q T}-1) = 41,\ (\beta_q)^q = 3.73E12,\ \Rightarrow$
Explicit stabilization penalty$=(B\epsilon/\omega)\times 1.1E-11$.

Error bounds for ill-posed $w_t = Lw,\ 0 \le t \le T$**.**

Noisy initial data f_δ, not exact f, with $\| f_\delta - f \|_2 \le \delta$.

Let $e(t_n) = w_{ex}(t_n) - w^n$, denote the error at $t_n = n\Delta t$.

With $B = \sup_t\{\| (-\Delta)^p w_{ex}(t) \|_2\}$, **Pure Explicit error**

$$\| e(t_n) \|_2 \le \delta e^{\beta_q t_n} + (B\epsilon/\omega)(e^{\beta_q t_n}-1)/(\beta_q)^q + O(\Delta t)$$

With prescribed L^2 bound $\| w_{ex}(T) \|_2 \le M$, choosing
$\beta_q = (1/T)\log(M/\delta),\ \Rightarrow$ **quasi optimal error bound:**

$$\| e(t_n) \|_2 \le M^{t_n/T}\delta^{(T-t_n)/T} + O(\Delta t) + \text{stabilization penalty.}$$

Quasi optimal error also in **compensated leapfrog**.

Linear autonomous selfadjoint analysis

Compensated pure explicit and leapfrog can perform well on limited but significant class of problems with **small** T, and small stabilization penalty.

Stablity in **time-reversed** problem $\Rightarrow$ Quasi-optimal results, within **fundamental uncertainty** $M^{(T-t)/T}\delta^{t/T}$.

Stabilizing pair (ϵ, p) for S_Δ located **interactively**.

Nonlinear problems

Explicit schemes **extremely advantageous** in multi-dimensional nonlinear problems on fine meshes.

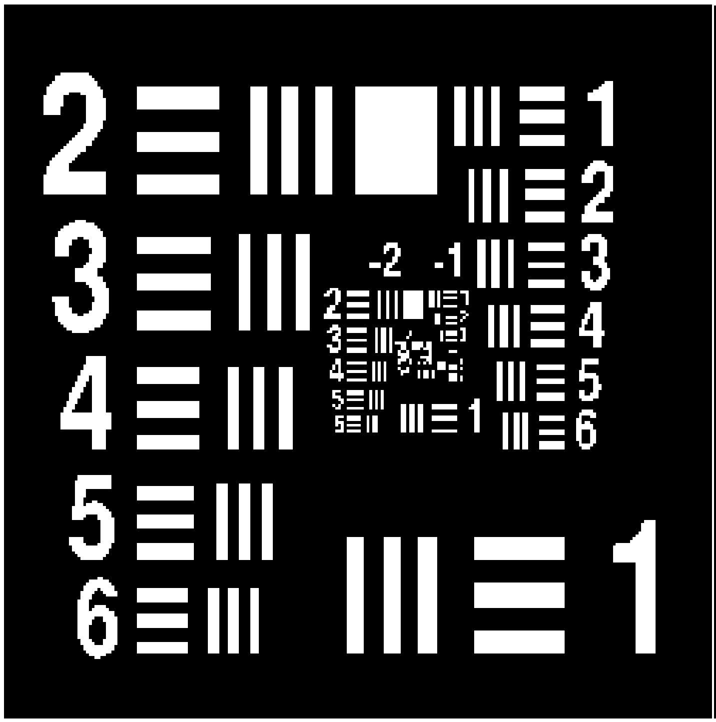
Laplacian smoother S_Δ effective with **nonlinear** L ???
Small stabilization penalty in nonlinear case ???
Stability in **nonlinear time-reversed** problems ???

FORWARD LEAPFROG COMPUTATION

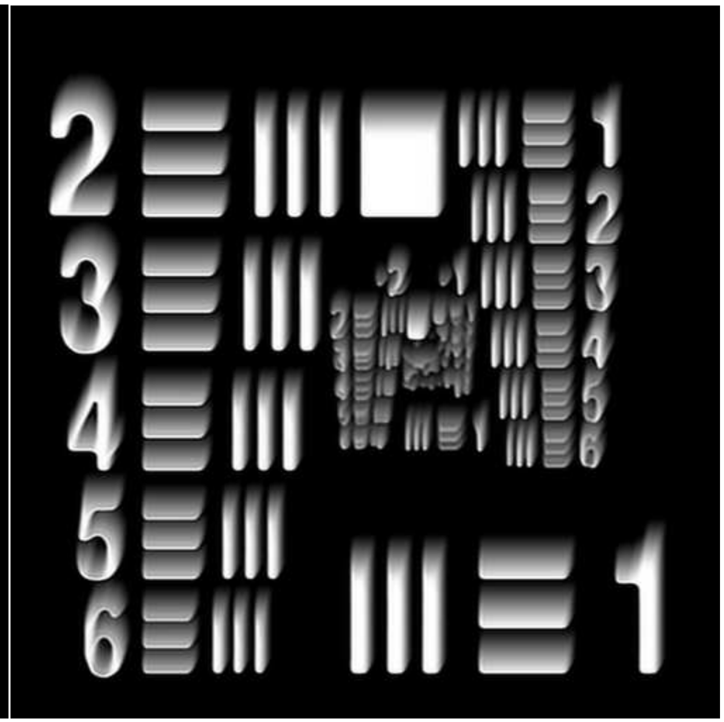
$$w_t = \exp(\sigma w)\nabla.\{q(x,y,t)\nabla w\} + c(w)w_x + d(w)w_y$$

STABILIZED LEAPFROG FORWARD TIME MARCHING IN LARGE ARRAY

Sharp 1024x1024 USAF chart image



Nonlinear parabolic leapfrog blur



Painless Leapfrog $O(\Delta t^2)$ computation. Crank-Nicholson $\Rightarrow$ solve **nonlinear** system of order 10^6 at each n.

TIME-REVERSED LEAPFROG COMPUTATION

$$w_t = \exp(\sigma w)\nabla.\{q(x,y,t)\nabla w\} + c(w)w_x + d(w)w_y$$

NONLINEAR LEAPFROG EXPERIMENT DONE ON SEPT 3 2015
SUCCESSFUL STABILIZED LEAPFROG FORWARD AND BACKWARD TIME MARCHING
IN NONLINEAR PARABOLIC EQUATION WITH VARIABLE TIME DEPENDENT COEFFICIENTS

SHARP JOAN CRAWFORD IMAGE

LEAPFROG NONLINEAR BLUR

LEAPFROG NONLINEAR DEBLUR

Moderate nonlinearity allows full leapfrog backward recovery, from $t = T$ to $t = 0$.

ONLY PARTIAL LEAPFROG RECOVERY

$$w_t = \mathrm{exp}(\sigma w)\nabla.\{q(x,y,t)\nabla w\} + c(w)w_x + d(w)w_y$$

Leapfrog nonlinear parabolic blurring of sharp 512x512 Joan Crawford image, with partial Leapfrog deblurring.

(Experiments performed on Sept 18 2015)

Nonlinear Parabolic Leapfrog Blur **30% Partial Leapfrog Deblur**

Stronger nonlinearity only allows partial leapfrog backward recovery, from $t = T$ to $t = 0.7T$.

LEAPFROG RECOVERY MAY FAIL AS $t \downarrow 0$.

$$w_t = \mathrm{exp}(\sigma w)\nabla.\{q(x,y,t)\nabla w\} + c(w)w_x + d(w)w_y$$

STABILIZED LEAPFROG SCHEME MARCHED BACKWARD IN TIME
Nonlinear parabolic blurring and deblurring of 512x512 image

INPUT BLURRED IMAGE t=T

PARTIAL DEBLURRING t= 0.7 T

PARTIAL DEBLURRING t= 0.6 T

PARTIAL DEBLURRING t= 0.5 T

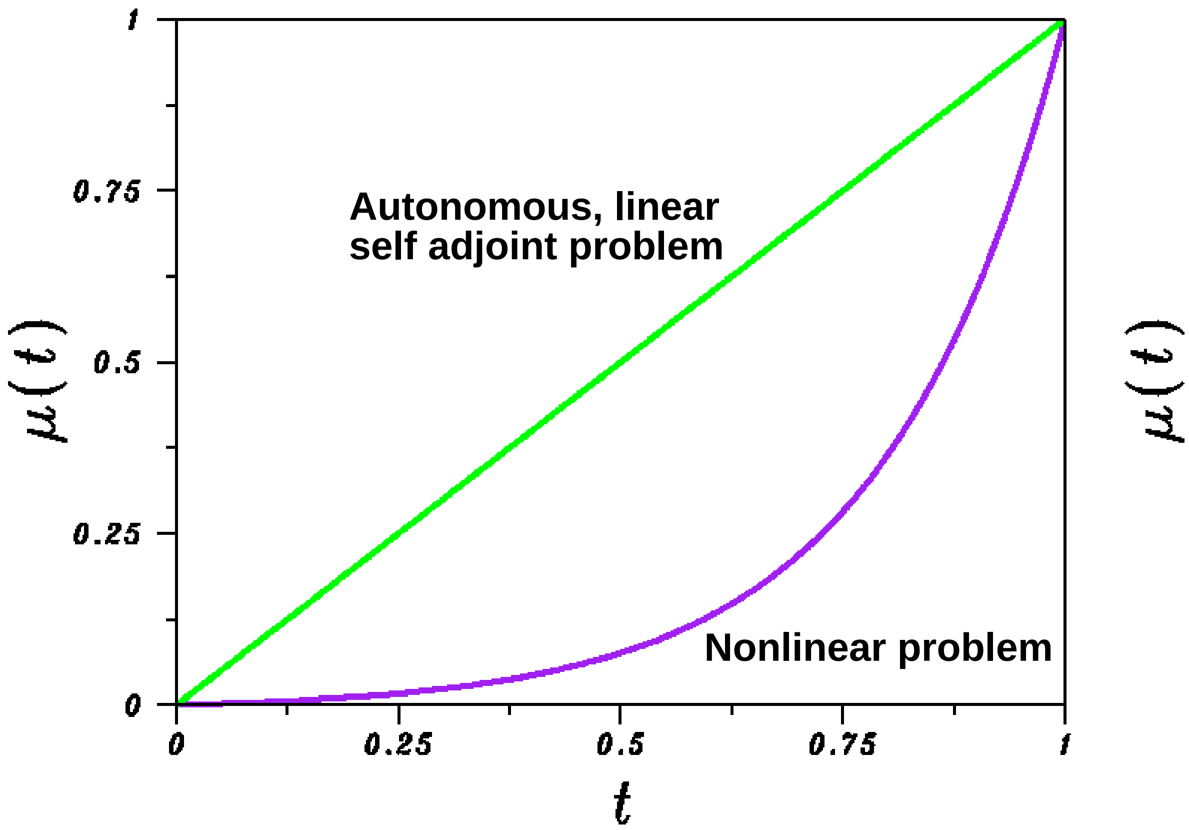
PARTIAL DEBLURRING t= 0.4 T

PARTIAL DEBLURRING t=0.2 T

Larger nonlinear uncertainty$= M^{1-\mu(t)}\delta^{\mu(t)}$, where $\mu(t) \downarrow 0$ exponentially as t decreases from $t = T$.

MAY NOT PERMIT FULL RECONSTRUCTION.

Behavior of Holder exponent in backward problems



PURE EXPLICIT SCHEME SURPRISE!

RECOVERS FROM BLURRED LEAPFROG DATA

$$w_t = \mathrm{exp}(\sigma w)\nabla.\{q(x,y,t)\nabla w\} + c(w)w_x + d(w)w_y$$

HEAVIER NONLINEAR LEAPFROG/EXPLICIT EXPERIMENT DONE ON SEPT 1 2015

LEAPFROG FORWARD TIME MARCHING FOLLOWED BY PURE EXPLICIT BACKWARD TIME MARCHING IN HEAVIER NONLINEAR PARABOLIC EQUATION

SHARP GENE TIERNEY IMAGE

AFTER LEAPFROG NONLINEAR BLUR

AFTER EXPLICIT NONLINEAR DEBLUR

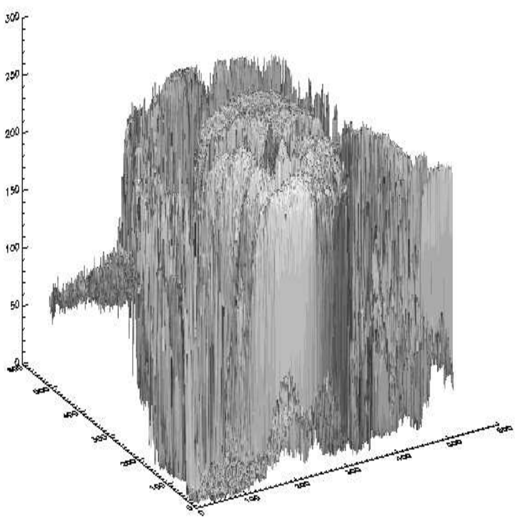
REMARKABLE DATA SURFACE RECOVERY

$$w_t = \exp(\sigma w)\nabla.\{q(x,y,t)\nabla w\} + c(w)w_x + d(w)w_y$$

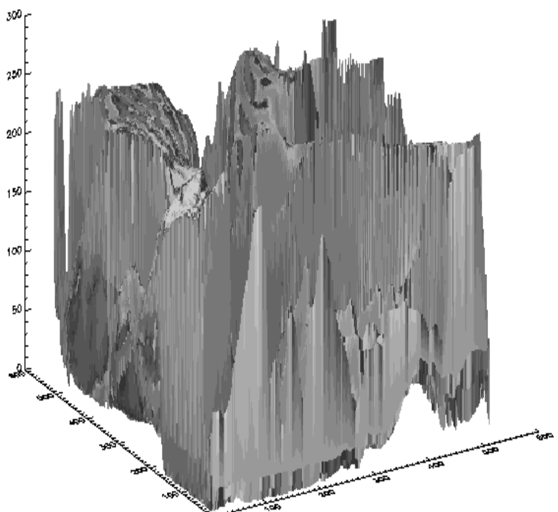
HEAVIER NONLINEAR LEAPFROG/EXPLICIT EXPERIMENT DONE ON SEPT 1 2015

LEAPFROG FORWARD TIME MARCHING FOLLOWED BY PURE EXPLICIT BACKWARD TIME MARCHING IN HEAVIER NONLINEAR PARABOLIC EQUATION

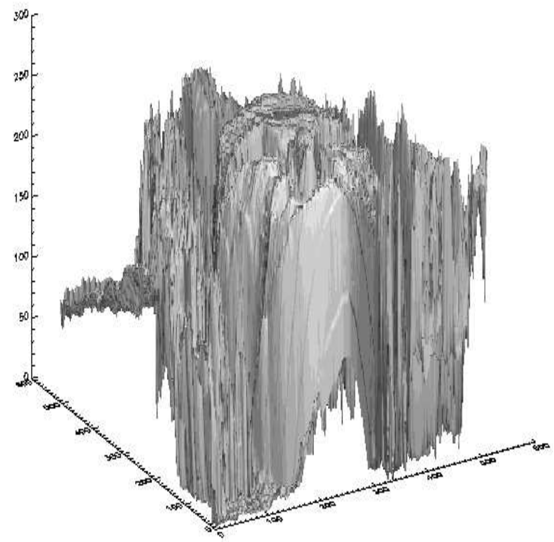
SHARP GENE TIERNEY DATA SURFACE



AFTER LEAPFROG NONLINEAR BLUR



AFTER EXPLICIT NONLINEAR DEBLUR



EXPLICIT RECOVERY FROM LEAPFROG.

$$w_t = \exp(\sigma w)\nabla.\{q(x,y,t)\nabla w\} + c(w)w_x + d(w)w_y$$

HEAVY NONLINEAR PDE BLURRING
USING STABILIZED LEAPFROG SCHEME

NONLINEAR PARTIAL DEBLURRING
USING STABILIZED EXPLICIT SCHEME

EXPLICIT RECOVERY FROM LEAPFROG.

$$w_t = \exp(\sigma w)\nabla.\{q(x,y,t)\nabla w\} + c(w)w_x + d(w)w_y$$

STABILIZED EXPLICIT FORWARD AND BACKWARD TIME MARCHING

Experiment done on July 14 2015

Nonlinear parabolic leapfrog blur

Pure explicit parabolic deblur

EXPLICIT RECOVERY FROM LEAPFROG.

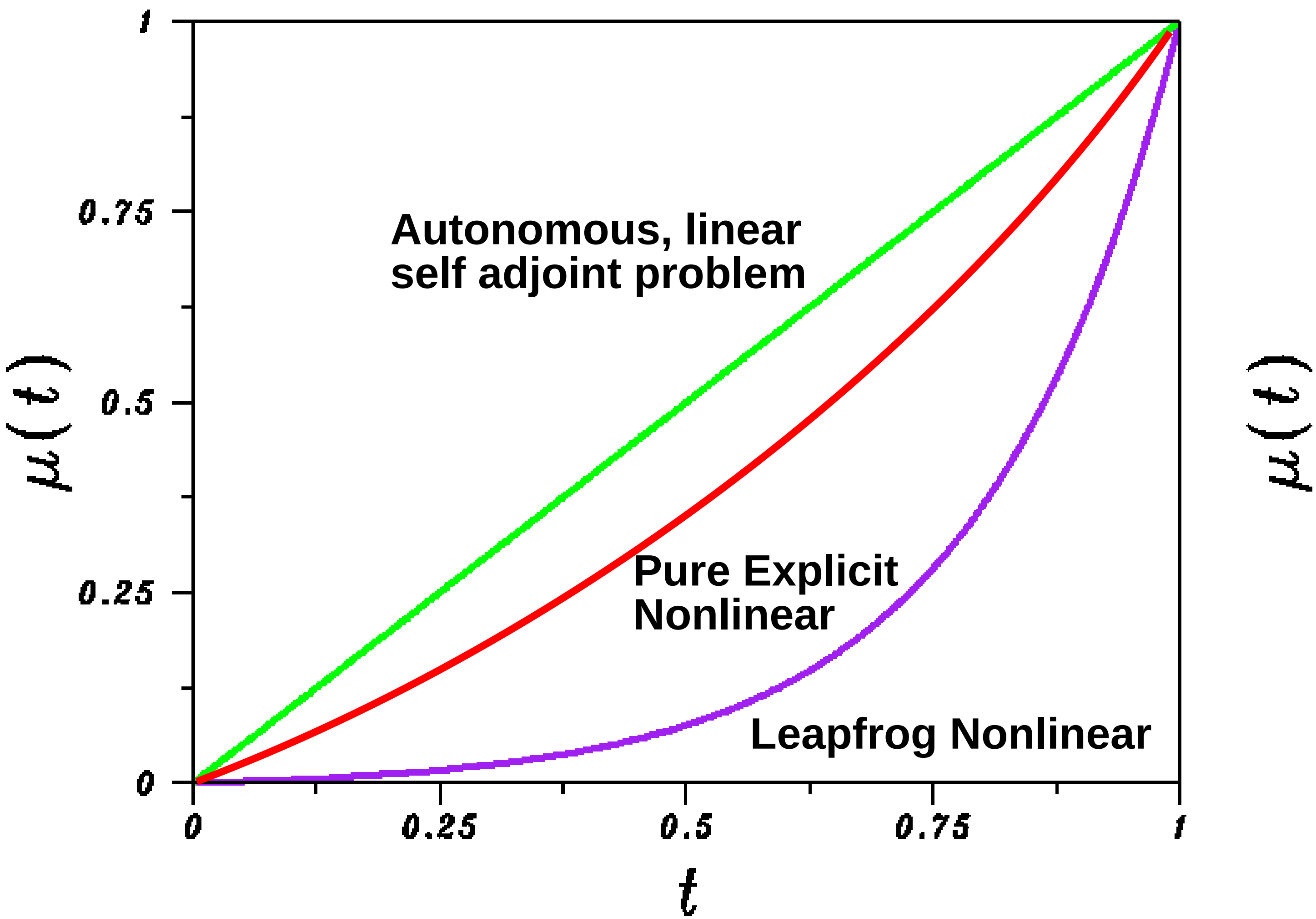
$$w_t = \mathsf{exp}(\sigma w)\nabla.\{q(x,y,t)\nabla w\} + c(w)w_x + d(w)w_y$$

HEAVY NONLINEAR PDE BLURRING
USING STABILIZED LEAPFROG SCHEME

NONLINEAR PARTIAL DEBLURRING
USING STABILIZED EXPLICIT SCHEME

UNEXPECTED PURE EXPLICIT ADVANTAGE

Behavior of Holder exponent in backward problems

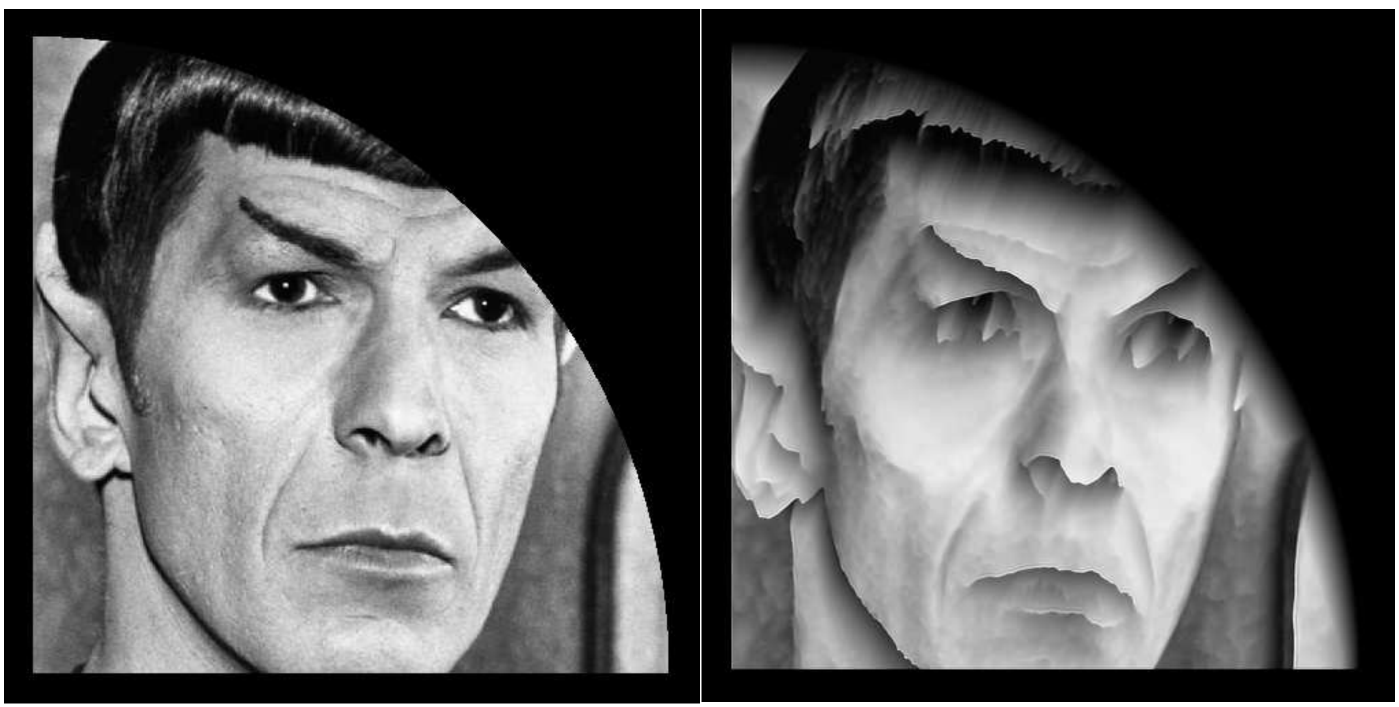


NON RECTANGULAR REGIONS Ω

Embed region Ω in larger square Γ.
At each $n\Delta t$, apply difference scheme inside Ω.
Extend computed solution by zero in $\Gamma - \Omega$.
Apply FFT-Laplacian smoothing operator S_{Δ} on Γ.
Return to Ω for next time step $(n+1)\Delta t$.

STABILIZED LEAPFROG FORWARD TIME MARCHING IN 1/4CIRCLE REGION
Quarter circle radius of 875 pixel embedded in 1024x1024 pixel array

At each n, PDE applied inside 1/4circle, extended by zero to whole square, then FFT Laplacian smoothed

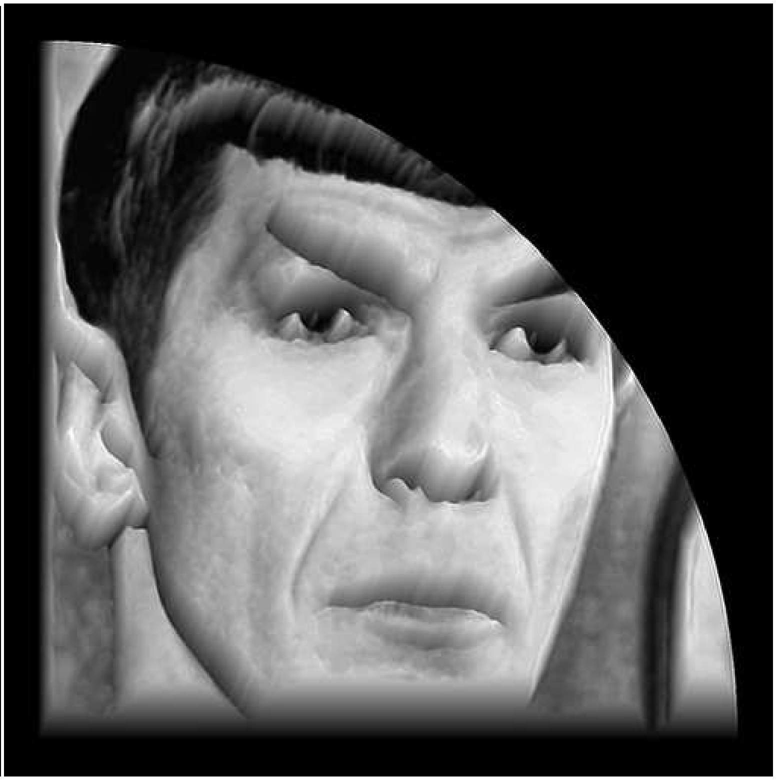


NON RECTANGULAR REGIONS Ω

Same strategy to march backward on Ω.

STABILIZED PURE EXPLICIT BACKWARD MARCHING IN 1/4CIRCLE REGION
1/4Circle region with radius 875 pixel is embedded in 1024x1024 pixel array

At each n, PDE applied inside 1/4circle, extended by zero to whole square, then FFT Laplacian smoothed



BACKWARD VISCOUS WAVE PROPAGATION

Constants $a, b > 0$, L positive selfadjoint elliptic,
$w_{tt} + aLw_t + bLw = 0 \quad t > 0; \quad w(0) = f, \quad w_t(0) = g.$

IRREVERSIBLE VISCOELASTIC WAVE PROPAGATION RUN BACKWARD IN TIME, USING STABILIZED EXPLICIT SCHEME.