simulation of selfsimilar rupture on nonuniform lattices

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Abstract

Project presentation at WIAS group – explaining efforts spend so far in implementation of the lubrication equation on nonuniform lattices.

Outline

1. simulation of rupture / model equation
2. discretization via Mathematica
3. refinement strategy
4. numerical results

1.1 Model

Equation for $x \in \Omega = (-1, 1)$ and $t \in [0, t^*)$:

$$\begin{aligned} h_t + (hu)_x &= 0 \\ \mathrm{Re}^*(u_t + uu_x) &= \frac{4}{h}(hu_x)_x + (3Sh_{xx} - \phi(h))_x - \frac{u}{bh} \end{aligned}$$

Boundary conditions (symmetry):

$$\begin{aligned} u(x+y,t) &= -u(x-y,t) && x \in \partial\Omega,\ \forall y \\ h(x+y,t) &= h(x-y,t) && x \in \partial\Omega,\ \forall y \end{aligned}$$

1.2 Comments

- boundary conditions retain symmetry of initial conditions

$$\begin{aligned} h_0 &= 1 - 0.2\cos(\pi x) \\ u_0 &= 0.1\sin(\pi x) \end{aligned}$$

- structure of differential operators allows for efficient inversion
- observation do not depend on initial conditions (h_0, u_0)
- a perturbation of $(1, 0)$ is then unstable if $S < 1/\pi^2$

1.3 Rupture

Observation:
There exists a finite-time singularity at (x^*, t^*) which has a self-similar structure.

That means:
There exists an $x^* \in \Omega$ such that $h(x^*, t) \to 0$ as $t \to t^*$ (from below). Close to (x^*, t^*) the solution (h, u) is of the form

$$h(x,t) = \tau^\alpha H(\eta), \qquad u(x,t) = \tau^\gamma U(\eta).$$

The self-similar variable η is defined by $\eta = (x - x^*)/\tau^\beta$ using $\tau = (t^* - t)$ the remaining time until the rupture.

1.4 Goal of simulation

Goal:
We want to determine solutions h, u near the singularity with such precision that we can determine α, β and γ and corresponding shape functions H and U with high precision. To exclude effects from transition we require that the simulation runs until

$$\min_x h(x,t) = O(10^{-10}).$$

For typical exponents $(\alpha = 1/3, \beta = 1/2, \gamma = -1/2)$ x is scaled by 10^{15}.

- double-precision ($\epsilon = 10^{-16}$) sufficient?
- fixed (nonuniform) lattice sufficient?

1.5 Implication for the simulation

Fixed lattice question:
One should pay attention to loss of significance. For example approximating a first derivative with difference quotient

$$\frac{h(x+a)-h(x)}{a} = h'(x) + O(a)$$

there is relative loss of significance $\epsilon h/(ah')$. Using a fixed nonuniform lattice we have a huge relative loss of significance where $a \approx \epsilon$ in the first stages of the simulation (i.e. for double-precision).

1.6 Implication for the simulation

Precision question:
Does loss of significance play a role if the lattice is *not* fixed?

No, if the lattice is chosen properly then small scales are absorbed in exponents of the double precision numbers and loss of significance is not amplified by too small lattice sizes.

2 Discretization

2.1 Iterative derivative

An example for a differential operator on a nonuniform lattice is

$$Df(x) = \frac{f(x+a) - f(x)}{a} + O(a(x)).$$

Note that $a = a(x)$ also depends on x. Is it a good idea to build higher order operators iteratively?

$$DDf(x) = \frac{1}{a(x+a)} \left(\frac{f(x+a+a(x+a)) - f(x+a)}{a(x+a)} - \frac{f(x+a) - f(x)}{a} \right) + O(?)$$

2.2 Iterative derivative

Answer:
Usually not, because . . .

1. iterative derivatives might increase size of difference star unnecessary,
2. do not have (sufficiently) high order,
3. scheme might even become inconsistent.

2.3 Iterative derivative

$$DDf(x) = \frac{1}{2}\left(1 + \frac{a(x+a)}{a}\right) f''(x) + O(a)$$

```
In[52]:= b = ξ * a;
         hm1 = h[x]; hi = h[x + a]; hp1 = h[x + a + b];
         SCHEME = a1 * hp1 + a2 * hi + a3 * hm1;
         a1 = 1 / (a * b);
         a2 = -1 / (a * b) - 1 / a^2;
         a3 = 1 / a^2;
         SER = Series[SCHEME, {a, 0, 1}];
         Expand[SCHEME, h]
         FullSimplify[SER]
```

Out[59]= $\frac{h[x]}{a^2} + \left(-\frac{1}{a^2} - \frac{1}{a^2\,\xi}\right) h[a+x] + \frac{h[a+x+a\,\xi]}{a^2\,\xi}$

Out[60]= $\frac{1}{2}\,(1+\xi)\,h''[x] + \frac{1}{6}\,(1+\xi)\,(2+\xi)\,h^{(3)}[x]\,a + O[a]^2$

Only if $a(x+a)/a = O(a)$, i.e. a very smooth lattice, the scheme is consistent.

2.4 Derivative via Mathematica

$$D^2 f(x+a) = \frac{2h(x)}{a(a+b)} - \frac{2h(x+a)}{ab} + \frac{2h(x+a+b)}{ab+b^2}$$

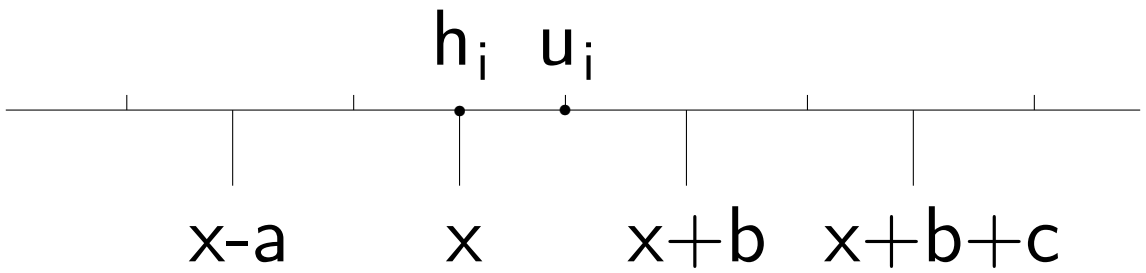
In[15]:=
```
b = ξ * a;
hm1 = h[x]; hi = h[x + a]; hp1 = h[x + a + b];
SCHEME = a1 * hp1 + a2 * hi + a3 * hm1;
SER = Series[SCHEME, {a, 0, 4}];
SOL = Solve[{SeriesCoefficient[SER, 0] == 0,
    SeriesCoefficient[SER, 1] == 0,
    SeriesCoefficient[SER, 2] == D[h[x], {x, 2}] / a^2},
   {a1, a2, a3}];
Expand[SCHEME /. SOL, h]
FullSimplify[SER /. SOL]
```

Out[20]= $\left\{\frac{2\,h[x]}{a^2\,(1+\xi)} - \frac{2\,h[a+x]}{a^2\,\xi} + \frac{2\,h[a+x+a\,\xi]}{a^2\,(\xi+\xi^2)}\right\}$

Out[21]= $\left\{h''[x] + \frac{1}{3}\,(2+\xi)\,h^{(3)}[x]\,a + \frac{1}{12}\,(3+\xi\,(3+\xi))\,h^{(4)}[x]\,a^2 + O[a]^6\right\}$

Here $D^2 f = h''(x) + O(a)$ holds. Centering can give an additional order.

2.5 Difference scheme for lubrication equation



Lattice 'points' in use:

$$h(x-a) = h_{i-1}, \quad h(x) = h_i, \quad h(x+b) = h_{i+1}, \quad h(x+a+b) = h_{i+2}$$

$$u(x-a/2) = u_{i-1}, \; u(x+b/2) = u_i, \; u(x+b+c/2) = u_{i+1}$$

2.6 Difference scheme for lubrication equation

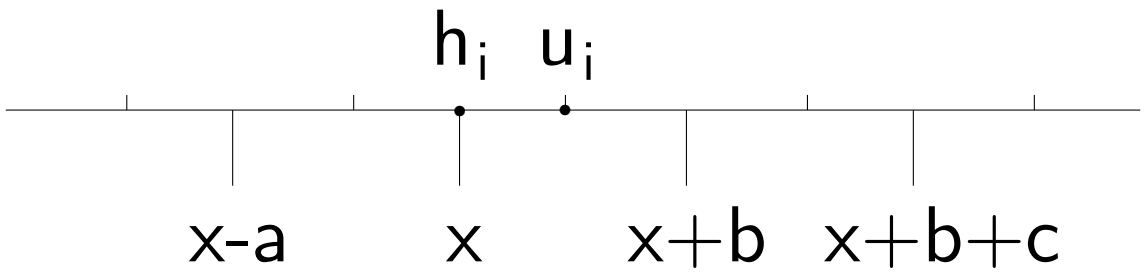
Explicit (example) of our discretization:

$$(hu)'(x) = \frac{\hat{h}(x+\frac{b}{2})u(x+\frac{b}{2}) - \hat{h}(x-\frac{a}{2})u(x-\frac{a}{2})}{(a+b)/2} + \frac{b-a}{4}\left[(hu)'' + h''u\right] + O(a^2)$$

via $\hat{h}(x+a/2) = (h(x)+h(x+a))/2$.

$$\begin{aligned} h^{(3)}(x+\frac{b}{2}) &= 6\left[\frac{h(x+b+c)}{c(b+c)(a+b+c)} - \frac{h(x+b)}{bc(a+b)} + \ldots \right. \\ &\quad \left. \frac{h(x)}{ab(b+c)} - \frac{h(x-a)}{a(a+b)(a+b+c)}\right] - \frac{1}{4}(c-a)h^{(4)} + O(a^2) \\ -\frac{h(x+b)^3 - h(x)^3}{b} &= \frac{3h'(x+\frac{b}{2})}{h^4(x+\frac{b}{2})} + \frac{20h'^3 - 12hh'h'' + h^2h^{(3)}}{8h^6}\, b^2 + O(b^3) \end{aligned}$$

2.7 On the boundary...



Boundary such that $x + b/2 = 1$: $u(x + b/2) \equiv 0$ and equation for $dh(x)/dt$ just involves $u(x - a/2)$, $u(x + b/2) \equiv 0$ and $h(x - a)$, $h(x)$, $h(x + b) = h(x)$ (symmetry condition). The other boundary is handled in the same way.

2.8 Open question

- The consistency is guaranteed by Taylor expansion for spatial derivatives (time stepping via implicit Euler method). done

- The stability of a nonlinear equation ($||(1 - \tau L(u, h))^{-1}|| < 1$) depends on solution and must be evaluated at different times $(h(\cdot, t), u(\cdot, t))$. There might also be a dependence on the refinement. not yet done

3 Refinement

3.1 Refinement goals

Strategy:
The primary aim is to obtain the significant part of the shape functions $H(\eta)$, $U(\eta)$ and the similarity scales α, β, γ. Therefor one has to identify the local x-scale dynamically. We use

$$a(x) = \min(C \left(\frac{h(x)}{h''(x)} \right)^{1/2}, h_{min})$$

where the constant is chosen $C \approx \sqrt{2e}$ with e being the (expected) relative local error.

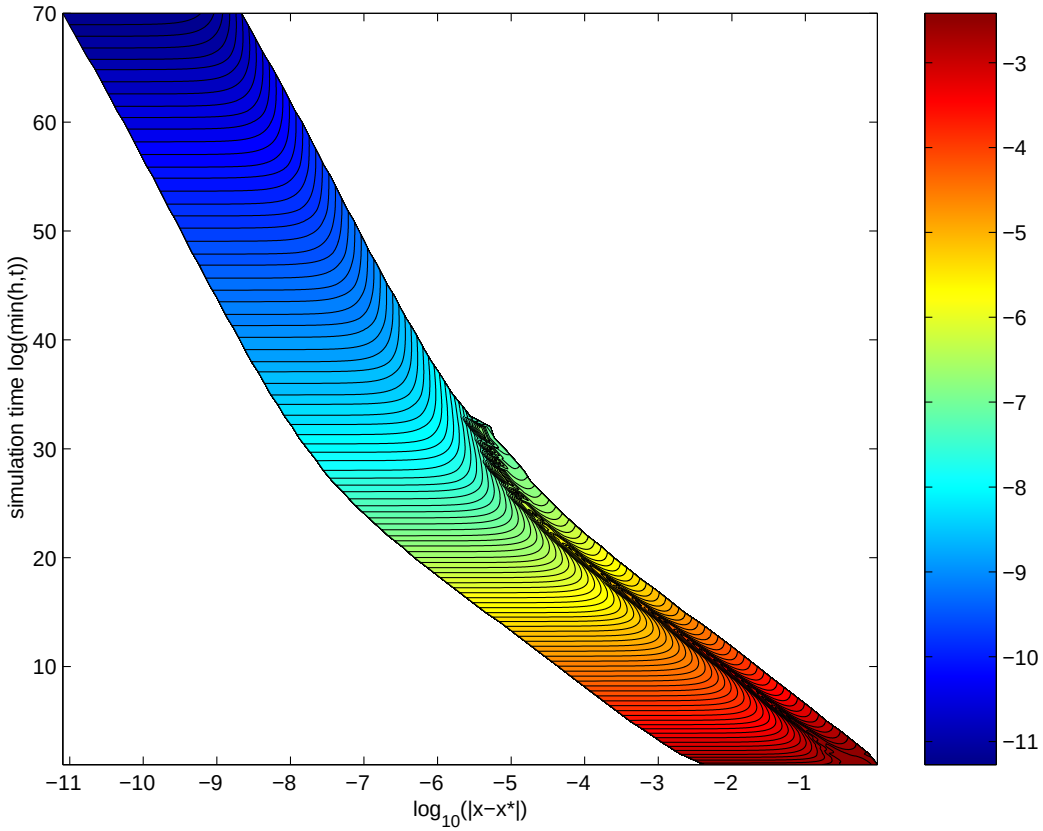
3.2 Note

Open question about the choice of $a(x)$:

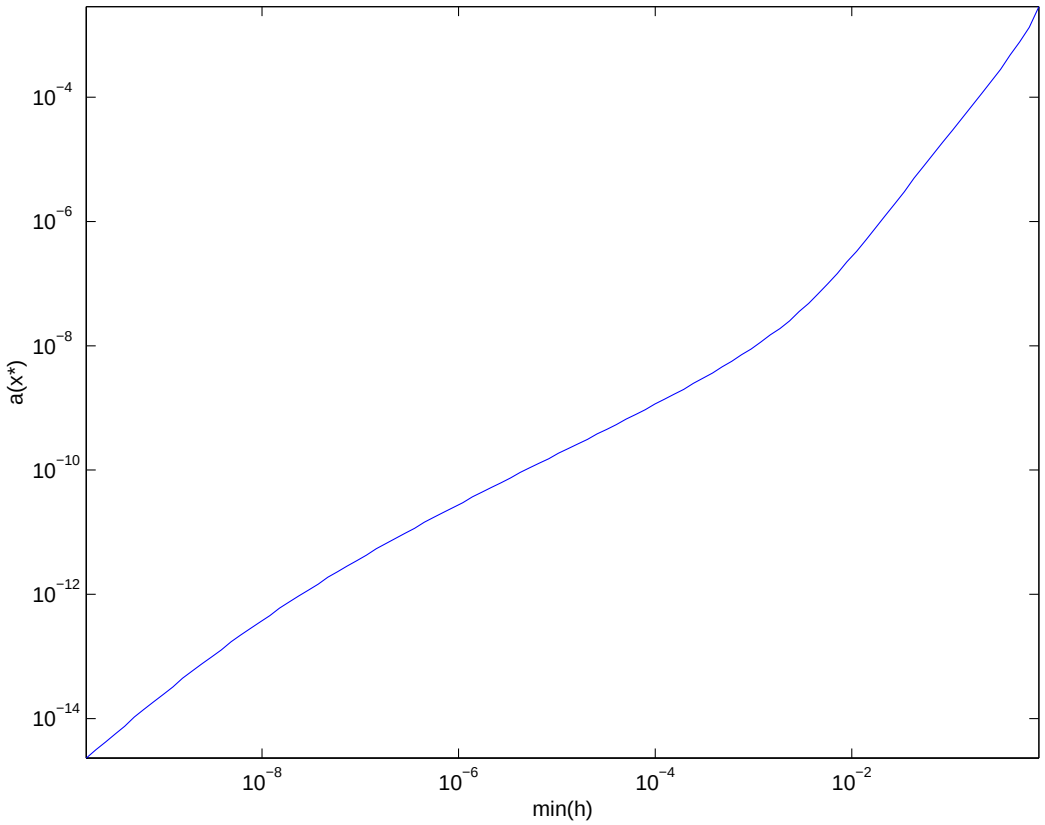
- can loss of significance really be neglected
- convergence of the solution with $e \to 0$
- one could also include higher (or lower) order terms or a velocity dependence

. . . but so far the methods has provided robust and reliable results.

3.3a Note


70
60
50
40
30
20
10
simulation time log(min(h,t))
−11
−10
−9
−8
−7
−6
−5
−4
−3
−2
−1
log10(|x−x*|)
−3
−4
−5
−6
−7
−8
−9
−10
−11

3.3b Note



3.4 Interpolation

- lattice update is done every m-th step (usually $m = 10$)
- to interpolate to new lattice cubic splines are used (algorithm Numerical recipes) with proper boundary conditions

4.1 Numerical results

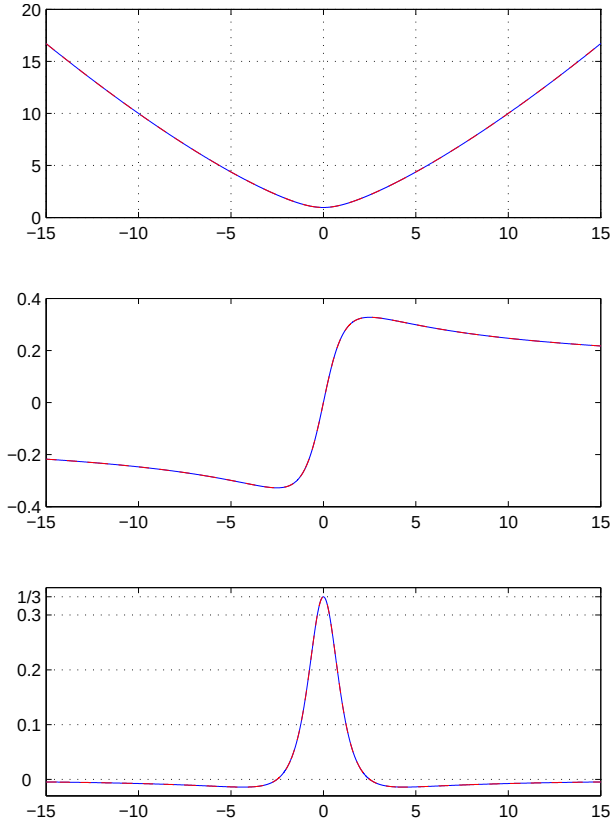


Figure 1: H, U and U' versus η

4.2 Numerical results

regime	α	β	γ	$H(\eta = 0)$
$L = 2,\ b = \infty$	0.333333	0.248930	-0.751070	0.96631
$L = 2,\ b = 1$	0.333333	0.248931	-0.751069	0.96629
$L = 5,\ b = 1$	0.333333	0.248931	-0.751070	0.96630
$L = 10,\ b = 1$	0.333333	0.248931	-0.751069	0.96630
init,$L = 2,\ b = 1$	0.333333	0.248930	-0.751070	0.96631

Table 1: numerical solutions with $Re^* = 0$, $b = 1$ and $S = 0.5/\pi^2$

Thank you for your attention!