A Splitting Scheme for Solving Reaction-Diffusion Equations Modelling Dislocatoin Dynamics in Materials Subjected to Cyclic Loading

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Summary

Posing the problem

Efects of applying cyclic loads to metals and alloys:

1. Breaking the uniform spatial distribution of dislocation;
2. Raise of local strains, dislocation cells, persistent slip bands, labyrinth structures of dislocations.

The Walgraef-Aifantis model (WA - 1985):

1. Reaction-duffusion, mesoscopic;
2. Two dislocation densities: static (dislocation forest) and mobile dsilocations.

The Walgraef-Aifantis model (WA)

Ref: *J. Appl. Phys.*, **58** (1985), 668

$$
\begin{aligned}
\frac{\partial \rho_s}{\partial t} &= D_s \nabla^2 \rho_s + \sigma - v_s d_c \rho_s^2 - \beta \rho_s + \gamma \rho_s^2 \rho_m \\
\frac{\partial \rho_m}{\partial t} &= \nabla_x \frac{1}{\gamma \rho_s^2} \nabla_x v_g \rho_m + \beta \rho_s - \gamma \rho_s^2 \rho_m
\end{aligned}
$$

where:

1. Time: measured in number of loading cycles;
2. ρ_s e ρ_m: Static and mobile dislocation densities;
3. σ: Constant rate of production of ρ_s;
4. *vs* e d_c: Critical velocity and critical distance for the colapse of a dislocation dipole;
5. β: Rate of conversion $\rho_s \longrightarrow \rho_m$;
6. γ: Rate of capture of mobile dislocations by a dipole;

Solving the WA model

1. Finite differences, second order in time, rectangular domain;
2. The target scheme - nonlinear
3. Achieving second order: internal iterations at each time step;
4. Decoupling raws and columns: splitting scheme (Stabilizing correction).

The target scheme

$$
\begin{aligned}
\frac{\rho_s^{n+1} - \rho_s^n}{\Delta t} &= \Lambda_x^{n+1/2} \frac{\rho_s^{n+1} + \rho_s^n}{2} + \Lambda_y^{n+1/2} \frac{\rho_s^{n+1} + \rho_s^n}{2} + f_1^{n+1/2} \\
\frac{\rho_m^{n+1} - \rho_m^n}{\Delta t} &= \Lambda_2^{n+1/2} \frac{\rho_m^{n+1} + \rho_m^n}{2} + f_2^{n+1/2}
\end{aligned}
$$

Main features:

1. Nonlinear, with two coupled equations;
2. Algebraic equations of lines coupled to the equations of columns: high computational cost;
3. The factor 2 is included in the definition of operators $\Lambda_x^{n+1/2}$, $\Lambda_y^{n+1/2}$ and $\Lambda_2^{n+1/2}$.

Internal iterations

$$\frac{\rho_s^{n+1,k+1} - \rho_s^n}{\Delta t} = \left(\Lambda_x^{n+1/2,k} + \Lambda_y^{n+1/2,k}\right) \frac{\rho_s^{n+1,k+1} + \rho_s^n}{2} + f_1^{n+1/2,k}$$

$$\frac{\rho_m^{n+1,k+1} - \rho_m^n}{\Delta t} = \Lambda_2^{n+1/2,k} \frac{\rho_m^{n+1,k+1} + \rho_m^n}{2} + f_2^{n+1/2,k}$$

Definition of operators – first equation

$$
\begin{aligned}
\frac{\partial \rho_s}{\partial t} &= D_s \nabla^2 \rho_s + \sigma - v_s d_c \rho_s^2 - \beta \rho_s + \gamma \rho_s^2 \rho_m \\
\frac{\rho_s^{n+1,k+1} - \rho_s^n}{\Delta t} &= \Lambda_x^{n+1/2,k} \frac{\rho_s^{n+1,k+1} + \rho_s^n}{2} + \\
&\quad \Lambda_y^{n+1/2,k} \frac{\rho_s^{n+1,k+1} + \rho_s^n}{2} + f_1^{n+1/2} \\
\Lambda_x^{n+1/2,k} &= \frac{D_s}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{4} v_s d_c \left(\frac{\rho_s^{n+1,k} + \rho_s^n}{2} \right) - \frac{\beta}{4} \\
\Lambda_y^{n+1/2,k} &= \frac{D_s}{2} \frac{\partial^2}{\partial y^2} - \frac{1}{4} v_s d_c \left(\frac{\rho_s^{n+1,k} + \rho_s^n}{2} \right) - \frac{\beta}{4} \\
f_1^{n+1/2,k} &= \sigma + \frac{\gamma}{2} \left(\frac{\rho_s^{n+1,k} + \rho_s^n}{2} \right)^2 \left(\rho_m^{n+1,k} + \rho_m^n \right) - \frac{\beta}{2} \rho_s^n
\end{aligned}
$$

Definition of operators – second equation

$$\frac{\partial \rho_m}{\partial t} = \nabla_x \frac{v_g}{\gamma \rho_s^2} \nabla_x v_g \rho_m + \beta \rho_s - \gamma \rho_s^2 \rho_m$$

$$\frac{\rho_m^{n+1,k+1} - \rho_m^n}{\Delta t} = \Lambda_2^{n+1/2} \frac{\rho_m^{n+1,k+1} + \rho_m^n}{2} + f_2^{n+1/2}$$

$$\Lambda_2^{n+1/2,k} = \frac{1}{2} \frac{\partial}{\partial x} \frac{1}{\gamma \left(\frac{\rho_s^{n+1,k} + \rho_s^n}{2} \right)^2} \frac{\partial}{\partial x} v_g - \gamma \left(\frac{\rho_s^{n+1,k} + \rho_s^n}{2} \right)^2$$

$$f_2^{n+1/2,k} = \beta \left(\frac{\rho_s^{n+1,k} + \rho_s^n}{2} \right)$$

The alternative scheme

The target scheme is replaced by an alternative one, featuring:

1. Iterative (linear), semi-implicit;
2. Stabilizing terms: implicit;
3. Destabilizing terms: explicit;
4. First equation $\longrightarrow$ replaced by two others *(splitting)*, to save memory and avoid large linear systems;
5. Splitting scheme: *Stabilizing Correction*, more stable than Alternating Directions – ADI (ref: Ianenko, N. N., *The Method of Fractional Steps*, Springer, 1971, Christov & Pontes, *Math. & Comp. Mod.*, **35**, *87-99, 2002*.

Splitting of the first equation

The original scheme of the first equation

$$\frac{\rho_s^{n+1,k+1} - \rho_s^n}{\Delta t} = \left(\Lambda_x^{n+1/2,k} + \Lambda_y^{n+1/2,k}\right) \frac{\rho_s^{n+1,k+1} + \rho_s^n}{2} + f_1^{n+1/2,k}$$

The equivalent scheme:

$$\frac{\tilde{\rho}_s - \rho_s^n}{\Delta t} = \Lambda_x^{n+1/2,k} \tilde{\rho}_s + 2\Lambda_y^{n+1/2,k} \rho_s^n + \Lambda_x^{n+1/2} \rho_s^n + f_1^{n+1/2}$$

$$\frac{\rho_s^{n+1,k+1} - \tilde{\rho}_s}{\Delta t} = \Lambda_y^{n+1/2,k} \left(\rho_s^{n+1,k+1} - \rho_s^n\right)$$

Main features of the scheme:

- Error of same order of the original;
- More stable than the original;
- Does not change the steady state solution.

Splitting of the first equation

The original scheme:

$$\frac{\rho_s^{n+1,k+1} - \rho_s^n}{\Delta t} = \left(\Lambda_x^{n+1/2,k} + \Lambda_y^{n+1/2,k}\right) \frac{\rho_s^{n+1,k+1} + \rho_s^n}{2} + f_1^{n+1/2,k}$$

The equivalent scheme:

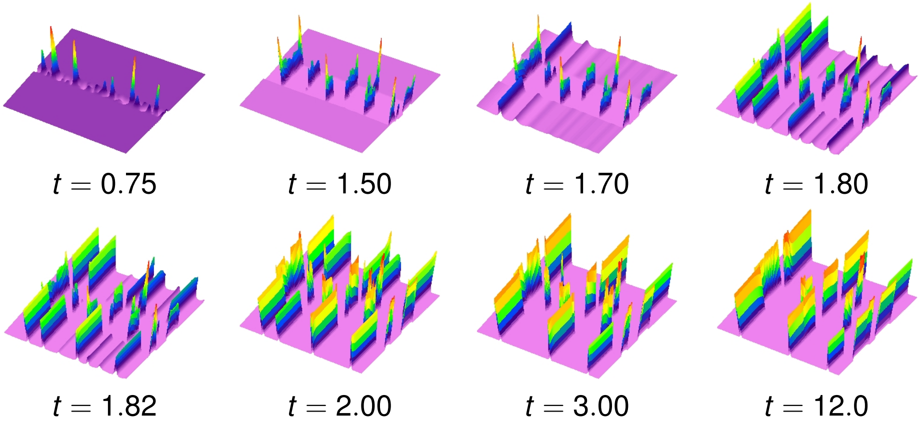
$$\left(I + \Delta t^2 \, \Lambda_x^{n+1/2i,k} \Lambda_y^{n+1/2,k}\right) \frac{\rho_s^{n+1,k+1} - \rho_s^n}{\Delta t} = \left(\Lambda_x^{n+1/2,k} + \Lambda_y^{n+1/2,k}\right) \frac{\rho_s^{n+1,k+1} - \rho_s^n}{2} + f_1^{n+1/2,k}$$

The scheme is equivalent to the original one, except for the positive operator with norm > 1:

$$B \equiv I + \Delta t^2 \, \Lambda_x^{n+1/2,k} \Lambda_y^{n+1/2,k} = I + \mathcal{O}\left(\Delta t^2\right)$$

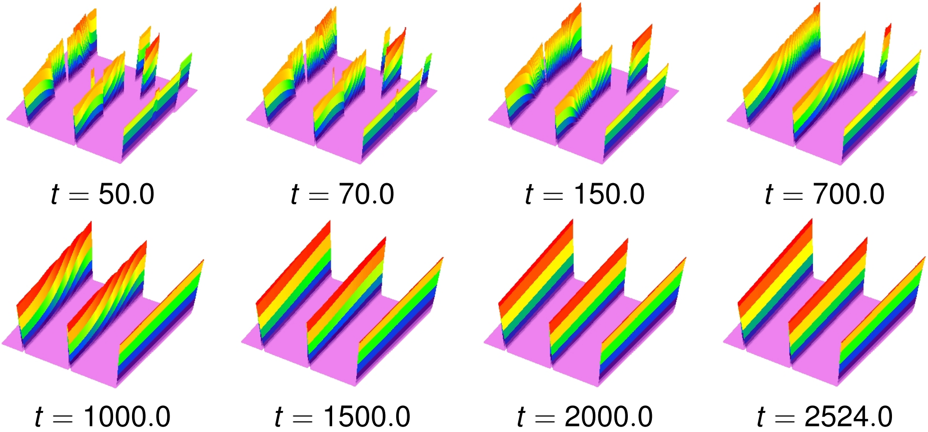
Results - linear diffusion of ρ_s

Time evolution of ρ_s



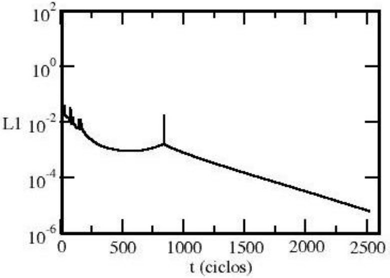
Results - linear diffusion of ρ_s

Time evolution of ρ_s – linear diffusion



Results - linear diffusion of ρ_s

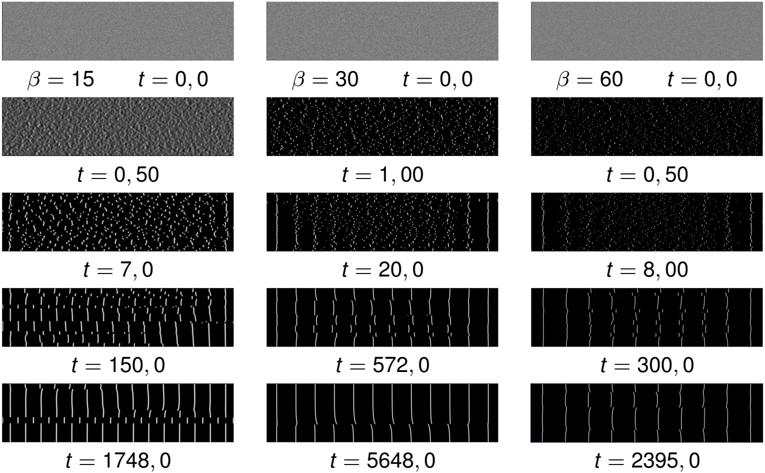
Rate of change of the distance between two successive states $\times t$



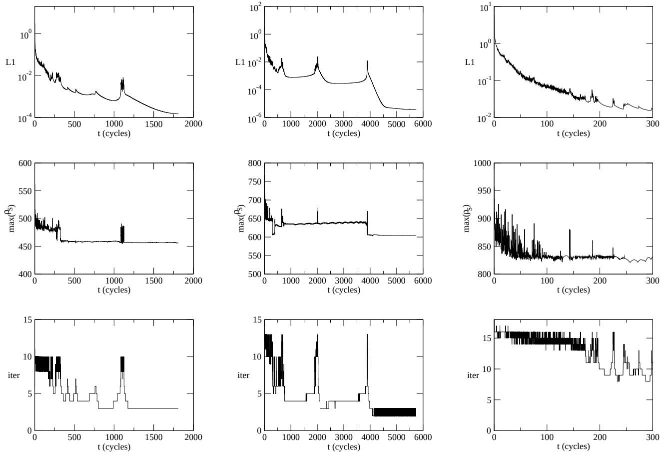
$$L_1 = \frac{1}{\Delta t}\frac{\sum_{ij}|\rho_s^{n+1} - \rho_s^n| + \sum_{ij}|\rho_m^{n+1} - \rho_m^n|}{\sum_{ij}|\rho_s^{n+1}| + \sum_{ij}|\rho_m^{n+1}|}$$

Results - nonlinear diffusion of ρ_s

Time evolution of ρ_s – nonlinear diffusion



Results - nonlinear diffusion of ρ_s



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