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# A Petrov–Galerkin transformation that eliminates spurious oscillations for heterogeneous diffusion–reaction equations

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## Abstract

In this paper a transformation technique is developed for diffusion–reaction equations of autocatalytic type, which possess spatially variable coefficients, that removes the possibility of spurious oscillations when using a backward Euler time discretization with large time steps. The approach can be considered as a construction of “special shape functions” yielding a stable Petrov–Galerkin type approximation. © 2001 Elsevier Science B.V. All rights reserved.

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## 1. Introduction

In many applications, diffusion–reaction equations with heterogeneous coefficients result from a consideration of a mass balance of a small diffusing species through an inhomogeneous medium (Fig. 1). As a model problem, we consider a structure which occupies an open bounded domain in  $\Omega \in \mathbb{R}^3$ , with boundary  $\partial\Omega$ . The boundary consists of  $\Gamma_c$  and  $\Gamma_G$ , where the solute concentrations, denoted by  $c$  (molecules/m<sup>3</sup>), and solute fluxes, denoted by  $\mathbf{G}$ , are respectively specified. The diffusive properties of the heterogeneous material are characterized by a spatially varying, symmetric, diffusivity tensor  $\mathbb{D} \in \mathbb{R}^{3 \times 3}$ , which is assumed to be bounded and positive-definite, i.e.,

$$\forall \nabla c \in \mathbb{R}^3, \quad a_+ \nabla c \cdot \nabla c \geq \nabla c \cdot \mathbb{D} \cdot \nabla c \geq a_- \nabla c \cdot \nabla c, \quad \infty > a_-, a_+ > 0 \quad \forall \mathbf{x} \in \Omega,$$

where  $D_{ij}(\mathbf{x}) = D_{ji}(\mathbf{x})$ ,  $1 \leq i, j \leq 3$ ,  $D_{ij}(\mathbf{x})$  being the Cartesian components of  $\mathbb{D}$  at point  $\mathbf{x}$ . We consider an arbitrary subvolume of material contained within  $\Omega$ , denoted  $\omega$ , consisting of a storage term ( $\dot{c}$ ), a reaction term ( $\dot{s}$ ), and an inward normal flux term ( $-\mathbf{G} \cdot \mathbf{n}$ ), leading to

$$\int_{\omega} (\dot{c} + \dot{s}) d\omega = - \int_{\partial\omega} \mathbf{G} \cdot \mathbf{n} da.$$

Typically, one assumes that the diffusing species reacts (is created or destroyed) in a manner such that the rate of production of the reactant ( $s$ ) is directly proportional to the concentration of the diffusing species

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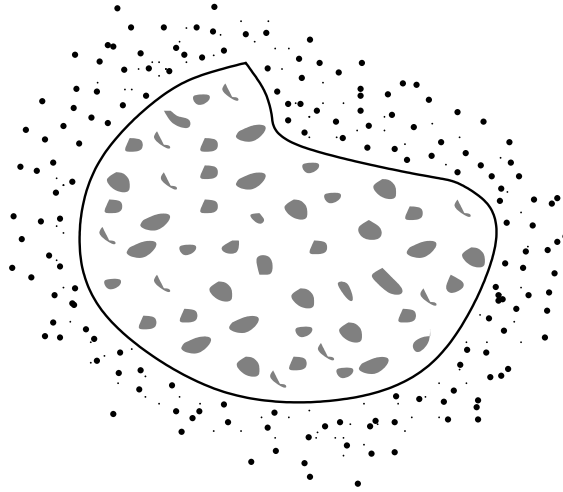


Fig. 1. Diffusion of a small species through a heterogeneous medium.

itself,  $\dot{s} = \tau c$  [1]. When  $\tau > 0$ , the diffusing species is destroyed as it reacts, while  $\tau < 0$  means that more of the diffusing species is produced as it reacts, i.e., an autocatalytic or “chain” reaction occurs. Upon substitution of these relations into the conservation law for the diffusing species, and after using the divergence theorem, since the volume  $\omega$  is arbitrary, one has the usual diffusion–reaction model in strong form  $\dot{c} = \nabla \cdot (\mathbb{D} \cdot \nabla c) - \tau c$ . A classical temporal approximation, that of Euler, is derived from a Taylor’s series expansion about time  $t^{L+1}$ ,

$$c^L = c^{L+1} - \left. \frac{\partial c}{\partial t} \right|_{t^{L+1}} (\Delta t) + \frac{1}{2} \left. \frac{\partial^2 c}{\partial t^2} \right|_{t^{L+1}} (\Delta t)^2 - \frac{1}{6} \left. \frac{\partial^3 c}{\partial t^3} \right|_{t^{L+1}} (\Delta t)^3 + \dots,$$

to give

$$\left. \frac{\partial c}{\partial t} \right|_{t^{L+1}} = \frac{c^{L+1} - c^L}{\Delta t} + \mathcal{O}(\Delta t).$$

Whenever time discretization is performed, one seeks methods with the property that, if errors made at one stage of the calculations, they do not cause increasingly larger errors as the computations are continued, but will eventually damp out, i.e., so-called *computational stability*. For the implicit backward Euler type approximation, there is an upper limit for the step size that can be used to retain computational stability, i.e., to avoid spurious growing oscillations. For example, consider the diffusion–reaction model in one dimension,

$$D \frac{d^2 c}{dx^2} - \tau c = \dot{c}.$$

Discretizing this equation with the implicit backward Euler scheme, and assuming, for the moment, that  $D$  and  $\tau$  are constants, then

$$D \frac{d^2 c^{L+1}}{dx^2} - \tau c^{L+1} = \frac{c^{L+1} - c^L}{\Delta t},$$

which implies

$$\frac{d^2 c^{L+1}}{dx^2} - \frac{1}{D} \left( \frac{1}{\Delta t} + \tau \right) c^{L+1} = -\frac{c^L}{D\Delta t}.$$

One observes that when  $\tau < 0$  the system is of nonoscillatory type only for small  $\Delta t$ . If  $\Delta t$  is too large  $\tau$ , will dominate, and the system will exhibit spurious, *coarse time-step induced*, oscillations. Therefore, for autocatalytic cases, the *upper limit* during time stepping is

$$\Delta t = \min_{x \in \Omega} \left| \frac{1}{\tau(x)} \right|.$$

Typically, in order to accurately resolve the heterogeneous material, use of very fine spatial discretization, for example finite element meshes, is unavoidable. Therefore, in order to reduce computation time, one would like to take as large time steps as possible. Thus, in attempt to use larger time steps, we consider a transformation technique which can eliminate spurious oscillations for diffusion–reaction equations involving autocatalytic reactions.

## 2. A transformation

Consider the following decomposition,

$$c = \hat{c} e^{-\tau t},$$

which is motivated by considering the pure reaction problem,  $\dot{w} = -\tau w$ , which has the solution of  $w = w_0 e^{-\tau t}$ . Classical transformations of this type can be found in Ames [2], *under the assumption that all material parameters are constant*. Inserting the approximation, we obtain  $\dot{\hat{c}} = \nabla \cdot (\mathbb{D} \cdot \nabla \hat{c})$ . Thus, the original equation is transformed into a standard diffusion equation, which can be dealt with by a standard backward Euler scheme, yielding stable results. *As already stated, such a transformation only holds if  $\tau$  is constant*. Thus, consider an alternative transformation,  $c = \hat{c} e^{-\tau^* t}$ , where  $\tau^*$  is a constant to be chosen later. Inserting this, we obtain,

$$\dot{\hat{c}} = \nabla \cdot (\mathbb{D} \cdot \nabla \hat{c}) - \underbrace{(\tau - \tau^*)}_{\zeta} \hat{c}. \quad (1)$$

On the continuum level, the objective would be to force

$$\zeta \stackrel{\text{def}}{=} \tau - \tau^* \geq 0$$

everywhere in the domain, which implies that we must choose  $\tau^* \leq \tau$ . However, in general  $\mathbb{D}$  is not differentiable, therefore we now consider weak formulations, which lead, in a natural way, to a finite element setting.

## 3. Weak form and temporal discretization

Following standard notation,  $H^1(\Omega)$  denotes the usual space of functions with generalized partial derivatives of order  $\leq 1$  in  $L^2(\Omega)$ . It is assumed that the boundary data are  $L^2(\partial\Omega)$  admissible, however, less smooth data can be considered without complications. Consider the following weak form for the untransformed field equation

Find  $c \in H^1(\Omega), c|_{\Gamma_c} = C$  such that  $\forall v \in H^1(\Omega), v|_{\Gamma_c} = 0$

$$\int_{\Omega} \nabla v \cdot \mathbb{D} \cdot \nabla c \, d\Omega = - \int_{\Omega} v \dot{c} \, d\Omega - \int_{\Omega} v \tau c \, d\Omega + \int_{\Gamma_G} v \mathbf{G} \cdot \mathbf{n} \, d\Omega \tag{2}$$

and the corresponding discrete form at a time step  $L + 1$

Find  $c^{L+1} \in H^1(\Omega), c^{L+1}|_{\Gamma_c} = C$  such that  $\forall v \in H^1(\Omega), v|_{\Gamma_c} = 0$

$$\int_{\Omega} \nabla v \cdot \mathbb{D} \cdot \nabla c^{L+1} \, d\Omega + \underbrace{\int_{\Omega} v \left( \frac{1}{\Delta t} + \tau \right) c^{L+1} \, d\Omega}_{\text{possibly negative}} = \frac{1}{\Delta t} \int_{\Omega} v c^L \, d\Omega + \int_{\Gamma_G} v \mathbf{G} \cdot \mathbf{n} \, dA. \tag{3}$$

Now consider the transformed equation

Find  $\hat{c} \in H^1(\Omega), \hat{c}|_{\Gamma_c} = C e^{\tau^* t}$  such that  $\forall v \in H^1(\Omega), v|_{\Gamma_c} = 0$

$$\int_{\Omega} \nabla v \cdot \mathbb{D} \cdot \nabla \hat{c} \, d\Omega = - \int_{\Omega} v \dot{\hat{c}} \, d\Omega - \int_{\Omega} v \zeta \hat{c} \, d\Omega + \int_{\Gamma_G} v e^{\tau^* t} \mathbf{G} \cdot \mathbf{n} \, d\Omega \tag{4}$$

and the corresponding discrete form at a time step  $L + 1$

Find  $\hat{c}^{L+1} \in H^1(\Omega), \hat{c}^{L+1}|_{\Gamma_c} = C e^{\tau^* t}$  such that  $\forall v \in H^1(\Omega), v|_{\Gamma_c} = 0$

$$\int_{\Omega} \nabla v \cdot \mathbb{D} \cdot \nabla \hat{c}^{L+1} \, d\Omega + \underbrace{\int_{\Omega} v \left( \frac{1}{\Delta t} + \zeta \right) \hat{c}^{L+1} \, d\Omega}_{\text{always positive}} = \frac{1}{\Delta t} \int_{\Omega} v \hat{c}^L \, d\Omega + \int_{\Gamma_G} v e^{\tau^* t} \mathbf{G} \cdot \mathbf{n} \, dA. \tag{5}$$

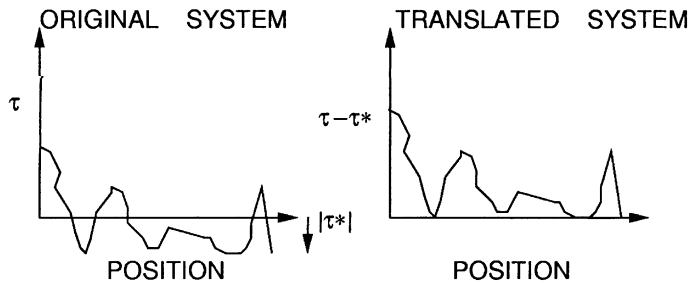


Fig. 2. Shifting the coefficient behavior.

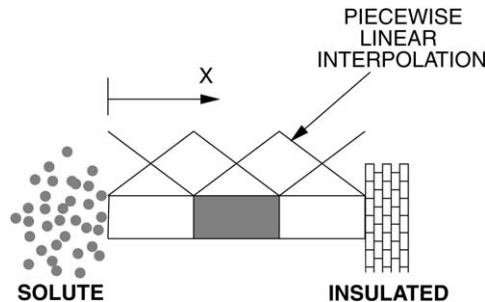


Fig. 3. An example with four piecewise (spatially) linear shape functions in the transformed system.

Table 1  
Diffusive properties

Material	$D$ (m <sup>2</sup> /s)	$\tau$ (1/s)
Matrix	0.000001	-0.00001
Particle	0.0000001	-0.0001

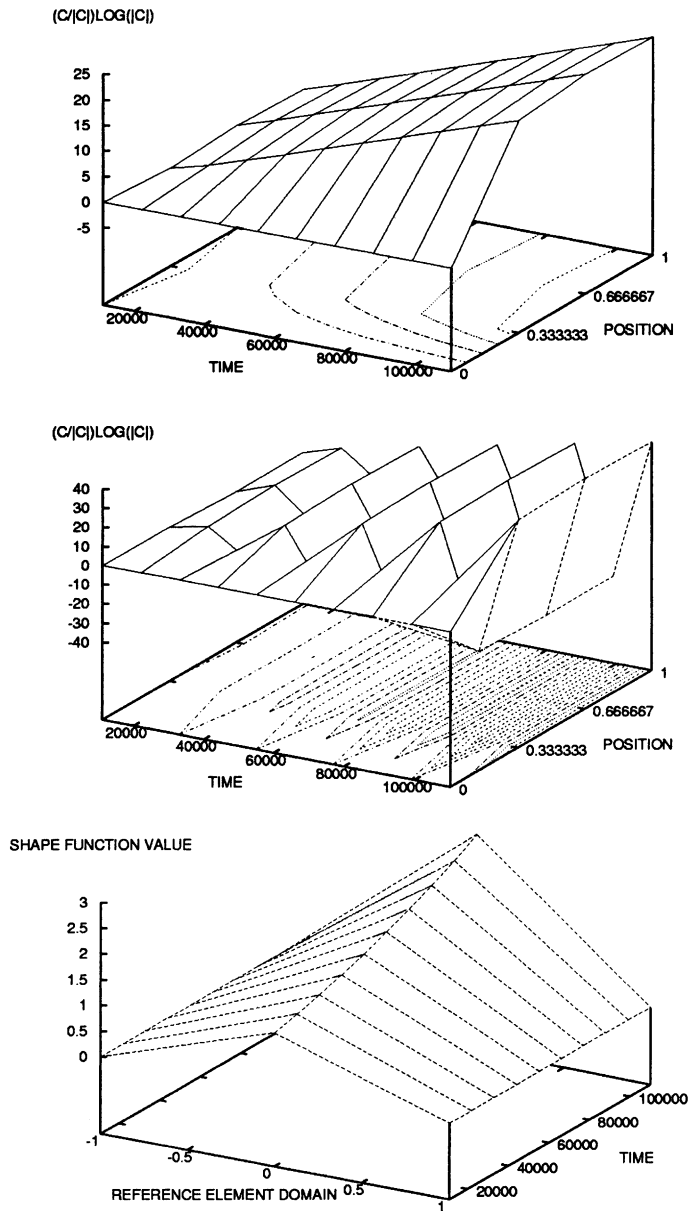


Fig. 4. Results (TOP) with a transformation and (MIDDLE) without any transformation. Also a “special” shape function’s behavior is depicted (BOTTOM) with growing time, over the referential element domain.

On the discrete level,  $\zeta$  is chosen such that  $(1/\Delta t) + \zeta \geq 0$  throughout the domain. As a by-product, this also insures that the corresponding stiffness matrix is positive definite. Furthermore, the resulting system remains symmetric, and thus standard iterative solvers, such as the Conjugate Gradient Method, can be employed.

**Remark 1.** If we use standard shape functions for the spatial discretization of the transformed system, then  $\hat{c} \approx \sum_{i=1}^N \hat{a}_i \phi_i(x_1, x_2, x_3)$ . Thus, one can interpret the different interpolations,  $c \approx e^{-\tau^* t} \sum_{i=1}^N \hat{a}_i \phi_i(x_1, x_2, x_3)$  and  $v \approx \sum_{i=1}^N b_i \phi_i(x_1, x_2, x_3)$  as a Petrov–Galerkin approximation.

**Remark 2.** Clearly, since we have the restriction that  $(1/\Delta t) + \zeta \geq 0$  throughout the domain, we must have at every point

$$\tau^* \leq \frac{1}{\Delta t} + \tau. \quad (6)$$

The logical choice for  $\tau^*$ , which by construction must be a constant, is  $\tau^* = \min_{\mathbf{x} \in \Omega} \tau(\mathbf{x})$ . This induces a shift, or “translation”, of the coefficient behavior of the system, as shown in Fig. 2. Such a shift will insure that the system remains positive definite even when using adaptive time stepping.

### 3.1. A numerical example

As an example consider a rod of unit length in Fig. 3, with  $c(0, t) = 1$ ,  $c(x, 0) = 0.1$  and  $G(L, t) = 0$  (Table 1). Shown in Fig. 4 are the stabilized and non-stabilized results for a time step size of  $\Delta t = 11\,000$  s,<sup>1</sup> which leads to  $\tau^* = -0.91 \times 10^{-5}$ . Also shown in Fig. 4 is a “special” shape function’s behavior with growing time depicted over the referential element domain  $[-1, 1]$ .

## 4. Final remarks

The transformation can be thought of as a “continuation” of a standard solution process into a (originally) spurious oscillation range, where large time steps are desired to be employed.

## References

- [1] J. Crank, in: *The Mathematics of Diffusion*, second ed., Oxford Science Publications, Oxford, 1975.
- [2] W.F. Ames, in: *Nonlinear Partial Differential Equations in Engineering*, Academic Press, New York, 1965.

<sup>1</sup> The choice of  $c(x, 0) = 0.1$  was simply to insure time-dependent solutions that were all positive.