# Fast Explicit Operator Splitting Method. Application to the Polymer System

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ABSTRACT. *Computing solutions of convection-diffusion equations, especially in the convection dominated case, is an important and challenging problem that requires development of fast, reliable numerical methods. We propose a second-order fast explicit operator splitting (FEOS) method based on the Strang splitting. The main idea of the method is to solve the parabolic problem via a discretization of the formula for the exact solution of the heat equation, which is realized using a conservative and accurate quadrature formula. The hyperbolic problem is solved by a second-order finite-volume Godunov-type scheme. The FEOS method is applied to the one- and two-dimensional systems modeling two phase multicomponent flow in porous media. Our results demonstrate that the method achieves a remarkable resolution and accuracy in a very efficient manner, that is, when only few splitting steps are performed.*

RÉSUMÉ. *Le calcul de solutions d'équations de type convection-diffusion est, specialement dans les cas où les effects convectifs dominent, un problème important et délicat qui requiert le développement de méthodes numériques rapides, précises et robustes. Nous proposons une méthode explicite d'ordre deux de type "operator splitting" basée sur la méthode du "Strang splitting". L'idée principale est de résoudre un problème parabolique via une discrétisation de l'expression de la solution exacte de l'équation de la chaleur par une méthode d'intégration numérique conservative. Le problème hyperbolique est résolu par un schéma volume finis de type Godunov d'ordre deux. La méthode est appliquée à des systèmes uni et bidimensionels modélisant des écoulements biphasiques en milieu poreux. Nos résultats établissent clairement la remarquable précision et efficacité de la méthode et le fait que seuls quelques pas de "splitting" sont nécessaires.*

KEYWORDS: *convection-diffusion equations, polymer system, operator splitting, finite-volume schemes, central-upwind schemes.*

*MOTS-CLÉS : equations convectives-diffusives, polymères, "operator splitting", schémas volumes finis, schémas centrés en amont.*

## 1. Introduction

We present a fast explicit operator splitting (FEOS) method for the initial value problem (IVP) for the system of convection-diffusion equations:

$$\mathbf{u}_t + \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{u}) = D\Delta\mathbf{u}, \qquad \mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d. \tag{1}$$

Here, $\mathbf{u}(\mathbf{x},t) = (u_1(\mathbf{x},t),\ldots,u_l(\mathbf{x},t))^T$ is an $l$-vector, $\mathbf{f}$ is a nonlinear convection flux, and $D = \mathrm{diag}(\varepsilon_1,\ldots,\varepsilon_l)$ is a constant diagonal matrix with positive entries.

Systems of convection-diffusion equations arise in a variety of applications and model different (physical) processes in fluid mechanics, astrophysics, meteorology, flow in porous media, and many other areas. In this paper, we consider systems that describe polymer flooding processes in enhanced oil recovery, see, for example, [JOH 88, RIS 91, TVE 90]. These systems are convection dominated, which is the most challenging case from a numerical perspective: although the solution of (1) is typically smooth for $t > 0$, its gradients may be very large and a full resolution of viscous shock layers may be out of practical reach. Therefore, an application of shock capturing methods, originally developed for hyperbolic systems of conservation laws may be advantageous. At the same time, even when the impact of diffusion is not too significant, its presence typically reduces the efficiency of explicit numerical schemes.

One way to overcome this difficulty is to use an operator splitting algorithm, which can be briefly described as follows. We denote by $\mathcal{S}_{\mathcal{H}}$ the *exact* solution operator associated with the corresponding hyperbolic system:

$$\mathbf{u}_t + \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{u}) = 0, \tag{2}$$

and by $\mathcal{S}_{\mathcal{P}}$ the *exact* solution operator associated with the (linear) parabolic system:

$$\mathbf{u}_t = D\Delta\mathbf{u}. \tag{3}$$

Then, introducing a time step $\Delta t$, the solution of the original convection-diffusion system (which is assumed to be available at time $t$) is evolved in time in three substeps:

$$\mathbf{u}(\mathbf{x}, t+\Delta t) = \mathcal{S}_{\mathcal{H}}(\Delta t/2)\mathcal{S}_{\mathcal{P}}(\Delta t)\mathcal{S}_{\mathcal{H}}(\Delta t/2)\mathbf{u}(\mathbf{x},t). \tag{4}$$

In general, if all solutions are smooth, this three-step splitting algorithm, called the Strang operator splitting, is second-order accurate (see, e.g., [STR 68]).

In practice, the exact solution operators $\mathcal{S}_{\mathcal{H}}$ and $\mathcal{S}_{\mathcal{P}}$ are replaced by their numerical approximations. Note that the main advantage of the operator splitting technique is the fact that the hyperbolic, (2), and the parabolic, (3), subproblems, which are of different nature, can be solved numerically by different methods.

The "hyperbolic" substep in our FEOS method is based on finite-volume schemes. Our particular choice is the second-order semi-discrete Godunov-type central scheme, originally introduced in [KUR 00b], and then further improved in [KUR 01], where the so-called *central-upwind* schemes have been developed. We note, however, that the "hyperbolic" substep is not tied up to a specific choice of a finite-volume scheme and can be implemented with one's favorite Godunov-type method.

The outcome of the first "hyperbolic" substep in (4) is a global approximation of $\mathbf{u}^* := \mathcal{S}_{\mathcal{H}}(\Delta t/2)\mathbf{u}(\mathbf{x},t)$, realized in terms of linear pieces over spatial cells. The main idea of our method is to perform the "parabolic" substep using the exact solution operator for the heat equation. The solution is in the form of a convolution integral, which is approximated using an appropriate conservative and sufficiently accurate quadrature, presented in §2.

In §3, we apply the FEOS method to the one- (1-D) and two-dimensional (2-D) polymer systems. The proposed FEOS method seems to outperform the existing alternative approaches.

## 2. Fast Explicit Operator Splitting (FEOS) Method

For simplicity, we present here only the 1-D version of the FEOS method. We introduce a uniform spatial grid of size $\Delta x$ and assume that the solution is known at time $t$.

The "hyperbolic" substep in (4) is carried out using a second-order Godunov-type finite-volume scheme, in which we begin with the computed cell averages

$$\bar{\mathbf{u}}_j(t) \approx \bar{\mathbf{u}}(x_j,t) := \frac{1}{\Delta x}\int\limits_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \mathbf{u}(x,t)\,dx.$$

The conservative piecewise linear (in $x$) interpolant for each component of the vector $\mathbf{u}$ is then reconstructed in each grid cell $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$ and is given by

$$\widetilde{\mathbf{u}}(x;t) = \bar{\mathbf{u}}_j(t) + \mathbf{s}_j(x - x_j), \tag{5}$$

where the slopes $\mathbf{s}_j$ have to be (at least) first-order approximations of the partial derivatives $\mathbf{u}_x(x_j,t)$. In order to ensure a non-oscillatory behavior of the reconstruction, which is a necessary condition for the overall scheme to be non-oscillatory, the slopes should be computed with the help of a nonlinear limiter (we have used the one-parameter family of minmod$\theta$ limiters, see, for example, [LIE 03, SWE 84]). Then, the solution at the new time level $t + \Delta t_{\mathrm{HYP}}$ is obtained by (approximately) solving the integral form of the system (2), subject to the piecewise linear initial data (5), prescribed at time $t$. In this paper, the solution is evolved using the semi-discrete central-upwind scheme from [KUR 01].

REMARK. — Note that due to the CFL condition, $\Delta t_{\rm HYP}$ may be smaller than $\Delta t/2$, where $\Delta t$ is the size of the splitting step. In this case, the "hyperbolic" substep of the splitting algorithm would consist of several smaller "finite-volume subsubsteps" of size $\Delta t_{\rm HYP}$. This is a typical situation, for example, in applications to polymer flows (see §3), where one is interested in developing a reliable operator splitting method that is capable to produce a high quality approximate solution with a small number of splitting steps, that is, while keeping $\Delta t$ relatively large.

Once the solution of the first "hyperbolic" substep in (4) is performed, the new cell averages, $\bar{\mathbf{u}}_j^* \approx \frac{1}{\Delta x}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \mathcal{S}_{\mathcal{H}}(\Delta t/2)\mathbf{u}(x,t)dx$, are available, and we reconstruct another piecewise linear interpolant $\widetilde{\mathbf{u}}^*(x)$ following (5). This piecewise linear function is then used as an initial condition for the parabolic IVP:

$$\mathbf{u}_t = D\mathbf{u}_{xx}, \qquad \mathbf{u}(x,t) = \widetilde{\mathbf{u}}^*(x), \tag{6}$$

which is now, according to the Strang splitting algorithm (4), to be solved on the time interval $(t, t+\Delta t]$. Note that since $D$ is a diagonal matrix, the parabolic system in (6) is actually a set of $l$ uncoupled heat equations for each component of $\mathbf{u}$:

$$(u_i)_t = \varepsilon_i (u_i)_{xx}, \qquad u_i(x,t) = \widetilde{u}_i^*(x), \quad i = 1,\ldots,l. \tag{7}$$

From now on, we will simplify our notation by using $v$ instead of any of the $u_i$'s and $\varepsilon$ instead of any of the $\varepsilon_i$'s.

Next, we recall that the exact solution of (7) at time $t+\Delta t$ may be expressed in the following integral form:

$$v^{**}(x) = \widetilde{v}^*(x) + \int_{-\infty}^{\infty} G(x-\xi, \varepsilon\Delta t)\left(\widetilde{v}^*(\xi) - \widetilde{v}^*(x)\right) d\xi, \tag{8}$$

where $G$ is the "heat" kernel:

$$G(x,t) = \frac{1}{2\sqrt{\pi t}} e^{-\frac{x^2}{4t}}. \tag{9}$$

We use the solution formula (8) since it is symmetric and allows us to discretize the spatial integral while preserving the conservation of $v$, that is, ensuring that the equality, $\int_{-\infty}^{\infty} v^{**}(x)\,dx = \int_{-\infty}^{\infty} \widetilde{v}^*(x)\,dx$, is satisfied on a discrete level as well.

Since for the next "hyperbolic" substep only the cell averages of $v^{**}(x)$ are needed, we average (8) over the corresponding computational cells to obtain:

$$\begin{aligned}
\bar{v}_j^{**} &= \bar{v}_j^* + \frac{1}{\Delta x}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \left[\int_{-\infty}^{\infty} G(x-\xi,\varepsilon\Delta t)\left(\widetilde{v}^*(\xi) - \widetilde{v}^*(x)\right) d\xi\right] dx \\
&= \bar{v}_j^* + \frac{1}{\Delta x}\sum_{i\in\mathbb{Z}} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} G(x-\xi,\varepsilon\Delta t)\left(\widetilde{v}^*(\xi) - \widetilde{v}^*(x)\right) d\xi\, dx.
\end{aligned} \tag{10}$$

Next, the integrals on the right-hand side (RHS) of (10) are discretized using the midpoint quadrature, that is,

$$\bar{v}_j^{**} = \bar{v}_j^{*} + \Delta x \sum_{i,\in\mathbb{Z}} G(x_j - x_i, \varepsilon\Delta t)(\bar{v}_i^{*} - \bar{v}_j^{*}). \tag{11}$$

It can be easily verified that this quadrature is conservative due to the symmetry of the "heat" kernel (9).

REMARK. — In practice, the computational domain is finite and the infinite sum on the RHS of (11) reduces to the sum over all computational cells (we obviously need to assume that the solution is "exponentially flat" near the artificially imposed boundaries).

The third and last substep of the FEOS method is again "hyperbolic". We start with the cell averages $\bar{\mathbf{u}}_j^{**}$, computed at the "parabolic" substep, reconstruct a piecewise linear interpolant $\hat{\mathbf{u}}$ (following (5)), and then evolve it using the same finite-volume method as in the first "hyperbolic" substep to obtain the cell averages of the solution of (1) at the new time level: $\bar{\mathbf{u}}_j(t+\Delta t) \approx \frac{1}{\Delta x}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \mathcal{S}_{\mathcal{H}}(\Delta t/2)\hat{\mathbf{u}}(x)\,dx$.

This completes the description of one time step of the FEOS method.

## 3. Application to the Polymer System

In this section, we apply the FEOS method to the 1-D and 2-D system of convection-diffusion equations that model polymer flooding processes in enhanced oil recovery (see [JOH 88, RIS 91, TVE 90] and the references therein). The initial data in our examples are taken form [KAR 01] and [HAU 01], and thus a comparison of our method with some existing alternative methods can be made.

### 3.1. *One-Dimensional Examples*

We first consider the 1-D system of two convection-diffusion equations:

$$\begin{cases} s_t + f(s,c)_x = \varepsilon s_{xx} \\ b_t + (cf(s,c))_x = \varepsilon b_{xx}, \end{cases} \tag{12}$$

with $b = b(s,c) = sc + a(c)$. Here, $(s,c)^T$ is the unknown state vector, $\varepsilon > 0$ is a small scaling parameter, and

$$f := f(s,c) = \frac{s2}{s2 + \mu(1+\nu c)(1-s)2}, \qquad a := a(c) = \frac{c}{5(1+c)}. \tag{13}$$

In the numerical experiments, presented in this section, we take $\mu = 1/2$ and $\nu = 2$.

We will compare the numerical solution computed by the FEOS method with a reference solution obtained without any operator splitting by combining the second-order

central-upwind scheme with the explicit second-order central-difference approximation of the diffusion term in (12). In our numerical experiments, we use the minmod1 limiter, since the flux here is nonconvex and, as it has been demonstrated in [KUR], the use of a more compressive minmod$\theta$ limiter with $\theta > 1$ may lead to a convergence to a "wrong" solution that does not satisfy the entropy condition for all entropies. This may not be a problem when $\varepsilon$ is large, but we are focusing on the convection dominated regime, in which a large error at the "hyperbolic" substep cannot be "fixed" by a small diffusion acting at the "parabolic" substep.

**Example 1**. Here, we consider the polymer system (12) subject to the following discontinues initial data:

$$(s,c)(x,0) = \begin{cases} (1.0, 0.5), & x \le 0.25, \\ (0.1, 0.1), & x > 0.25. \end{cases} \tag{14}$$

In the inviscid case, these initial data correspond to a Riemann problem, whose solution consists of an $s$-shock, followed by a $c$-shock and an $s$-rarefaction wave.

In Figure 1, we plot the approximate solutions of (12),(14) (dotted line) at time $t = 1$ for $\varepsilon = 0.001$ and $\varepsilon = 0.01$, computed by the FEOS method with two splitting steps and 500 uniform grid cells. The solid line represents a reference solution computed with 10000 cells. As one can clearly see, for $\varepsilon = 0.001$ the computed solution agrees well with the reference one, while for $\varepsilon = 0.01$ the $s$-component of the solution is smeared. Therefore, one needs to perform more than two splitting steps. In Figure 2, the solutions computed for $\varepsilon = 0.01$ by the FEOS method with 8 and 32 splitting steps are shown. Now the resolution of both $s$ and $c$ fronts is very high.

We also numerically study the convergence rate of the FEOS method with respect to the number of splitting steps. In order to do this, we fix the spatial mesh to 1000 uniform cells and increase the number of splitting steps. We then compute the relative $L^1$ errors and convergence rates, which are shown in Table 1. As one can see, the convergence rates start decreasing after a certain number of splitting steps. This occurs since the "heat" kernel (9) develops a singularity as $\Delta t \to 0$, and thus the splitting step in the FEOS method cannot be taken too small. A similar convergence study was performed in [KAR 01] and we would like to point out that the relative errors obtained in the FEOS method are, on the average, ten times smaller than those obtained in [KAR 01] (we refer the reader to that work for comparison).

**Example 2**. This example is a Riemann problem corresponding to a compressive shock in the inviscid case, in which both the $s$- and the $c$-characteristics go into a shock and contribute to its self-sharpening. The initial condition is given by

$$(s,c)(x,0) = \begin{cases} (0.75, 0.8), & x \le 0.25, \\ (0.839619, 0.4), & x > 0.25. \end{cases} \tag{15}$$

If this Riemann problem is slightly perturbed, the solution changes from a single shock to a composition of waves moving with almost the same speed (see, e.g., [KAR 01]).

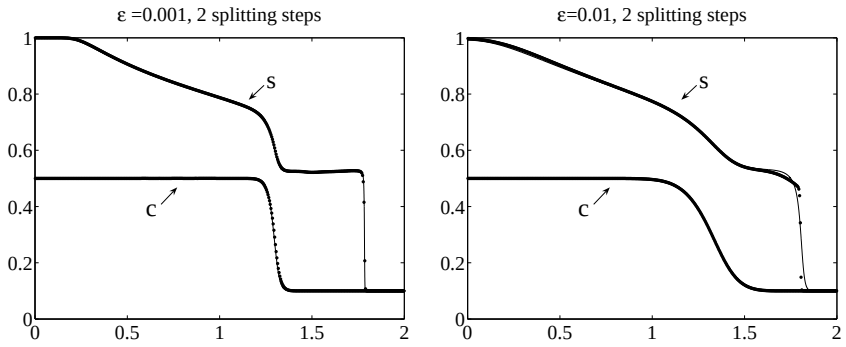


**Figure 1.** *Solution of (12),(14) with* $\varepsilon = 0.001$ *and* $\varepsilon = 0.01$ *by the FEOS method with 2 splitting steps (dotted line). The solid line represents the reference solution.*

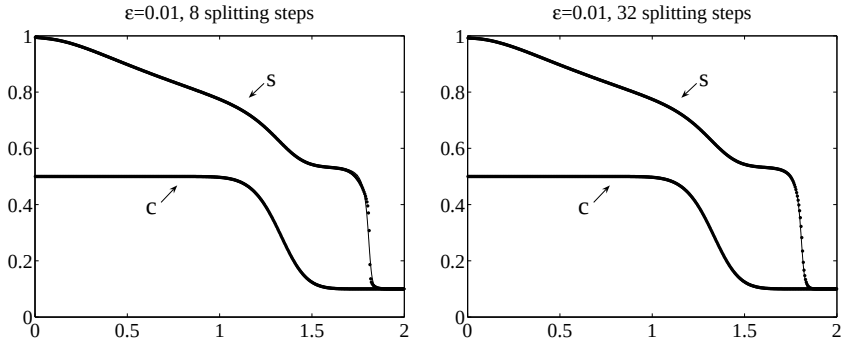


**Figure 2.** *Solution of (12),(14) with* $\varepsilon = 0.01$ *by the FEOS method with 8 and 32 splitting steps (dotted line). The solid line represents the reference solution.*

There are two possible results of the perturbation: either a monotone or a nonmonotone solution. In the viscous case, the problem will be perturbed instantly, which results in a truly nonlinear phenomenon: monotone initial data evolve into nonmonotone solutions. In Figure 3, we plot the approximate solutions of (12),(15) with $\varepsilon = 0.005$ (dotted lines) at time $t = 1$, computed by the FEOS with four splittings steps. As in the previous Example, we compare these solutions computed with 500 uniform grid cells with the corresponding reference solutions computed with 10000 cells. The exact (reference) solution has a dip in the $s$-component due to the presence of the diffusion term. As one can observe, the dip is not resolved well when four splitting steps are performed. Therefore, we also show the results obtained with 8 and 32 splittings steps, where a very high resolution is achieved. We would like to point out that the alternative operator splitting methods, described in [KAR 01], fail to resolve the dip in the $s$-component of the solution (see Figures 10 and 11 in [KAR 01]).

| Number of steps | $s$-component | | | | $c$-component | | | |
|---|---|---|---|---|---|---|---|---|
| | $\varepsilon = 0.001$ | | $\varepsilon = 0.01$ | | $\varepsilon = 0.001$ | | $\varepsilon = 0.01$ | |
| | $L^1$-error | Rate | $L^1$-error | Rate | $L^1$-error | Rate | $L^1$-error | Rate |
| 2 | 2.53e-03 | – | 8.80e-03 | – | 7.06e-04 | – | 3.28e-03 | – |
| 4 | 1.66e-03 | 0.61 | 5.94e-03 | 0.57 | 5.33e-04 | 0.41 | 1.87e-03 | 0.81 |
| 8 | 1.09e-03 | 0.61 | 3.47e-03 | 0.78 | 4.11e-04 | 0.38 | 9.25e-04 | 1.02 |
| 16 | 7.74e-04 | 0.49 | 1.57e-03 | 1.14 | 3.34e-04 | 0.30 | 3.96e-04 | 1.23 |
| 32 | 6.14e-04 | 0.33 | 5.96e-04 | 1.40 | 3.28e-04 | 0.02 | 1.45e-04 | 1.44 |
| 64 | 5.56e-04 | 0.14 | 2.07e-04 | 1.52 | 3.54e-04 | -0.11 | 4.31e-05 | 1.75 |
| 128 | 5.20e-04 | 0.09 | 9.05e-05 | 1.19 | 3.77e-04 | -0.09 | 2.01e-05 | 1.10 |
| 256 | 5.14e-04 | 0.01 | 7.38e-05 | 0.30 | 3.92e-04 | -0.05 | 2.58e-05 | -0.36 |

**Table 1.** *Example 1. Estimated errors and convergence rates for the $s$-and $c$-components of the solution, computed by the FEOS method at time $t = 1$.*

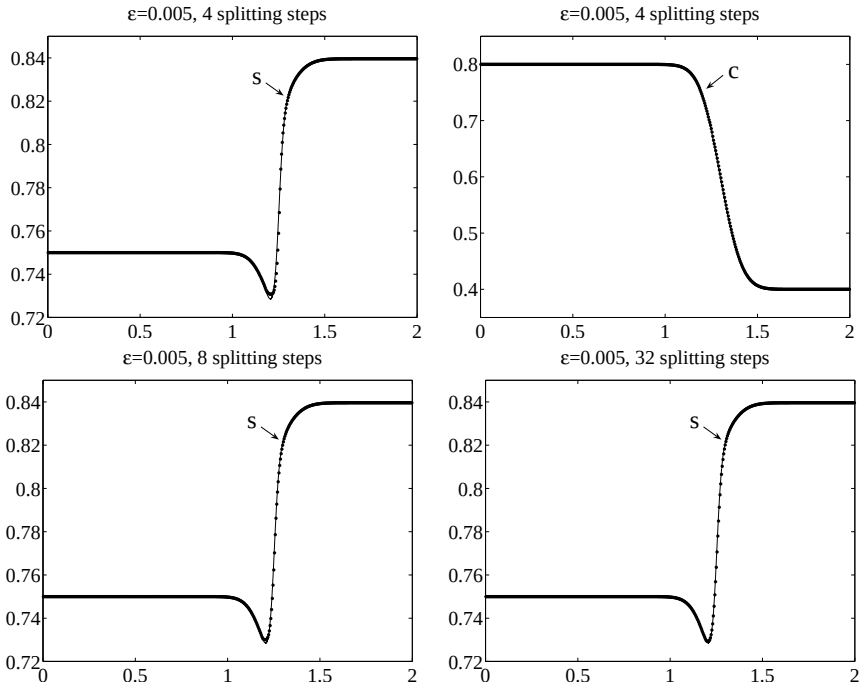


**Figure 3.** *Solution of (12),(15) with $\varepsilon = 0.005$ by the FEOS method with 4, 8, and 32 splitting steps (dotted line). The solid line represents the reference solution.*

### 3.2. *Two-Dimensional Example*

Finally, we consider the 2-D polymer system:

$$\begin{cases} s_t + f(s,c)_x + f(s,c)_y = \varepsilon(s_{xx} + s_{yy}) \\ b_t + (cf(s,c))_x + (cf(s,c))_y = \varepsilon(b_{xx} + b_{yy}), \end{cases} \tag{16}$$

where, as in the 1-D case, $b = b(s,c) = sc + a(c)$ and $f$ and $a$ are given by (13). We now take $\mu = \nu = 1$ and consider the 2-D Riemann problem with the initial data:

$$(s,c)(x,y,0) = \begin{cases} (1.0, 0.0), & x < 0,\ y < 0, \\ (1.0, 0.1), & x > 0,\ y > 0, \\ (0.0, 0.0), & \text{otherwise.} \end{cases} \tag{17}$$

The example is taken from [HAU 01], where the corresponding inviscid system was numerically solved by a front tracking method. Here, we consider the viscous case with $\varepsilon = 0.01$. The solutions, computed at time $t = 0.4$ by the FEOS method with $400 \times 400$ grid cells and two and four splitting steps, are plotted in Figure 4. As one can see, all major waves are already accurately captured with four splittings steps for the $s$-component of the solution and with only two steps for the $c$-component of the solution.

It should be pointed out that a fast and efficient implementation of the FEOS method in two (and more) dimensions can only be achieved by taking into account the special form of the heat kernel given by (9). The presence of exponents of type $e^{-\frac{(x_j - x_i)2 + (y_k - y_\ell)2}{4\varepsilon\Delta t}}$ on the RHS of (11), used in the "parabolic" substep of the FEOS method, allows one to perform the summation only in a (relatively) small neighborhood of each cell. This significantly reduces CPU times and thus makes the FEOS method very efficient.

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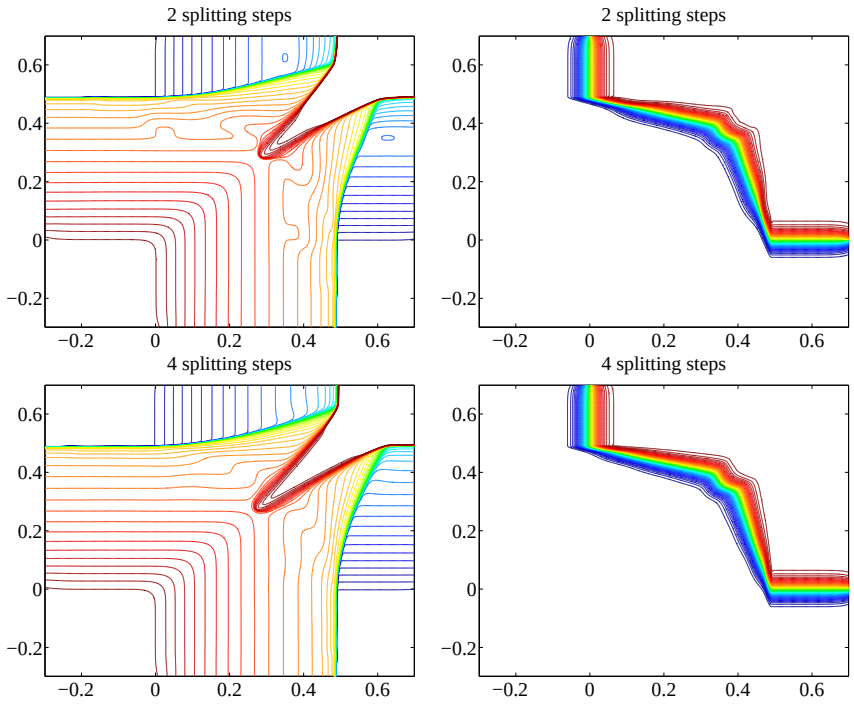


**Figure 4.** *$s$ (left) and $c$ (right) components of the solution of (16)–(17) with $\varepsilon = 0.01$ computed by the FEOS method on a $400 \times 400$ grid with 2 and 4 splitting steps.*

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