Mixed Collocation
for Fractional Differential Equations

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This contribution is dedicaced to Claude Brézinski
at the occasion of his sixtieth birthday.

Abstract
We present the mixed collocation method for numerical integration of fractional differential equations of the type $D^\beta u = \Phi\,(u,\, t)$. Given a regular mesh with constant discretization step, the unknown $u(t)$ is considered as continuous and affine in each cell, and the dynamics $\Phi(u,\, t)$ as a constant. After a fractional integration, the equation is written strongly at the mesh vertices and the dynamics weakly in each cell. The "Semidif" software has been developed for the particular case of numerical integration of order $\frac{1}{2}$. The validation for analytical results and published solutions is established and experimental convergence as the mesh size tends to zero is obtained. Good results are obtained for a nonlinear model with a strong singularity.

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1) Introduction

• Let β be a real number, $0 < \beta < 1$, $\Gamma(\bullet)$ the classical Euler function, and $\mathbb{R} \times [0, \infty[\ \ni (u, t) \longmapsto \Phi(u, t) \in \mathbb{R}$ a regular mapping. Following for example the now classical work of Caputo [Ca67], we define the fractional differential operator $D^\beta(\bullet)$ by

$$(1) \qquad (D^\beta u)(t) \equiv \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{\mathrm{d}u}{\mathrm{d}\theta} \frac{\mathrm{d}\theta}{(t-\theta)^\beta} \,.$$

We wish to approximate the "initial value problem" for the fractional ordinary differential equation of order β :

$$(2) \qquad \begin{cases} D^\beta (u - u_0) = \Phi(u(t), t) \,, & t > 0 \\ u - u_0 = 0 \,, & t \leq 0 \,. \end{cases}$$

• We introduce a discretization step h, and denote by $K^h_{j+\frac{1}{2}}$ the interval of the form $K^h_{j+\frac{1}{2}} \equiv \,]\, t^j \,, t^{j+1} \,[\ = \,]\, jh \,, (j+1)\, h\, [$ for $j \in \mathbb{N}$. We use the discrete spaces P_1^h and Q_0^h defined as follows. The linear space P_1^h is composed by functions that are continuous and affine in each mesh element $K^h_{j+\frac{1}{2}}$. A function $v \in P_1^h$ can be expanded on the basis $\big(\varphi_k^h\big)_{k \in \mathbb{N}}$ of classical "hat" functions :

$$\varphi_0^h(\theta) = \begin{cases} 1 - \dfrac{\theta}{h} \,, & 0 \leq \theta \leq h \\ 0 \,, & \theta \geq h \end{cases}$$

$$\varphi_k^h(\theta) = \begin{cases} 1 - \dfrac{1}{h}\big(\theta - t^k\big) \,, & t^k \leq \theta \leq t^{k+1} \,, \\ 1 + \dfrac{1}{h}\big(\theta - t^k\big) \,, & t^{k-1} \leq \theta \leq t^k \,, \qquad k \geq 1 \,, \\ 0 \,, & |\, \theta - t^k \,| \geq h \end{cases}$$

and by using the nodal values $v_k \equiv v\big(t^k\big)$ at the grid vertices, we have : $v = \sum_{k=0}^\infty v_k \, \varphi_k^h$ for $v \in P_1^h$.

• The discrete space Q_0^h is composed by functions that take a constant value in each element $K^h_{j+\frac{1}{2}}$. The basis functions of the discrete space Q_0^h are null everywhere except inside the interval $K^h_{j+\frac{1}{2}}$ where it is equal to the unity. Then, $w \in Q_0^h$ can be expanded on the $\chi^h_{k+\frac{1}{2}}$ basis according to the relation $\quad w = \sum_{k=0}^\infty w_{k+\frac{1}{2}} \ \chi^h_{k+\frac{1}{2}}$.

2) Mixed collocation scheme

• We integrate the differential equation (2) with the fractional integrator I^β of order β defined by

$$I^{\beta}\left(v\left(\bullet\right),t\right) \;\equiv\; \frac{1}{\Gamma\left(\beta\right)}\int_{0}^{t}\left(t-\theta\right)^{\beta-1}v\left(\theta\right)\,\mathrm{d}\theta$$

and satisfying the functional equation $I^{\beta}\circ D^{\beta}\equiv \mathrm{Id}$ when applied for a regular function u satisfying $u(0)=0$. The relation (2) can therefore be rewritten as

$$(3)\qquad u\left(t\right)-u_{0} \;=\; I^{\beta}\left(\Phi\left(u\left(\bullet\right),t\right)\right),\quad t\geq 0\,.$$

- The $P_1 Q_0$ mixed collocation method consists in choosing a discrete state $u^h\left(\bullet\right)$ satisfying

$$(4)\qquad u^{h}=\sum_{j=0}^{\infty}u_{j}^{h}\;\varphi_{j}^{h}\,,\qquad u^{h}\in P_{1}^{h}\,,$$

and the so-called "flux" $\Phi\left(u\left(\bullet\right),t\right)$ by a discontinuous time function $f^h(\bullet)$ that is constant in each cell $K^h_{j+\frac{1}{2}}$:

$$(5)\qquad f^{h}=\sum_{j=0}^{\infty}f_{j+\frac{1}{2}}^{h}\;\chi_{j+\frac{1}{2}}^{h}\,,\qquad f^{h}\in Q_{0}^{h}\,.$$

- On one hand, the equation (3) is written strongly at the mesh vertices jh $(j\in\mathbb{N})$ and we can speak of a **collocation** method :

$$(6)\qquad u^{h}\left(jh\right)-u_{0} \;=\; I^{\beta}\left(f^{h}\left(\bullet\right),jh\right)\,,\quad j\in\mathbb{N}\,.$$

On the other hand, it is a method inspired from **mixed** finite elements. We can not impose that for each time value t, we have $f^h(t)=\Phi(u^h(t),t)$. Then the $P_1 Q_0$ mixed collocation method claims only that for the mean values, the approached flux $f^h\left(\bullet\right)$ and the exact flux $\Phi\left(u^h\left(\bullet\right),\bullet\right)$ of the approached solution have the same mean value in each interval $]jh,(j+1)h[$. We impose :

$$\int_{jh}^{(j+1)h}f^{h}\left(\theta\right)\,\mathrm{d}\theta \;=\; \int_{jh}^{(j+1)h}\Phi\left(u^{h}\left(\theta\right),\theta\right)\,\mathrm{d}\theta\,,\qquad j\in\mathbb{N}\,.$$

This "projection step" on the discrete space Q_0^h can be written as :

$$(7)\qquad f_{j+\frac{1}{2}}^{h}=\int_{0}^{1}\Phi\left(u_{j}^{h}\left(1-\theta\right)+\theta u_{j+1}^{h},\;jh+\theta h\right)\mathrm{d}\theta\,,\qquad j\in\mathbb{N}\,.$$

Proposition 1. State-flux constraint for the $P_1 Q_0$ scheme
With the choice (4) (5), the relation (6) can be written in the following way :

$$(8)\qquad u_{j+1}^{h}-\frac{h^{\beta}}{\Gamma\left(\beta+1\right)}\,f_{j+\frac{1}{2}}^{h} \;=\; u_{0}+\frac{h^{\beta}}{\Gamma\left(\beta+1\right)}\sum_{k=0}^{j-1}\alpha_{j-k}\;f_{k+\frac{1}{2}}^{h}\,,\quad j\in\mathbb{N}\,,$$

with

$$\alpha_k \;\equiv\; (k+1)^{\beta} \,-\, k^{\beta}\,, \quad k \in \mathbb{N}\,. \tag{9}$$

Proof of proposition 1.

We evaluate the right hand side of relation (6) for the discrete time t^{j+1}. We have :

$$\begin{aligned}
I^{\beta}\left(f^{h}(\bullet)\,,t^{j+1}\right) \;&=\; \frac{1}{\Gamma(\beta)} \int_0^{t^j+1} \left(t^{j+1}-\theta\right)^{\beta-1} \, f^{h}(\theta)\,\mathrm{d}\theta \\
&=\; \frac{1}{\Gamma(\beta)} \sum_{k=0}^{j} \int_{kh}^{(k+1)h} (t^{j+1}-\theta)^{\beta-1} \, f^{h}(\theta)\;\mathrm{d}\theta \\
&=\; \frac{1}{\Gamma(\beta)} \sum_{k=0}^{j} f^{h}_{k+\frac{1}{2}} \int_0^1 [(j+1)^h-(kh+h\xi)]^{\beta-1} h\;\mathrm{d}\xi \\
&=\; \frac{1}{\Gamma(\beta)} \sum_{k=0}^{j} f^{h}_{k+\frac{1}{2}}\, h^{\beta} \left(\frac{-1}{\beta}\right) \left[(j+1-k-\xi)^{\beta}\right]_{\xi=0}^{\xi=1} \\
&=\; \frac{1}{\Gamma(\beta+1)} \sum_{k=0}^{j} f^{h}_{k+\frac{1}{2}}\, h^{\beta} \left[(j+1-k)^{\beta}-(j-k)^{\beta}\right] \\
&=\; \frac{h^{\beta}}{\Gamma(\beta+1)} \sum_{k=0}^{j} f^{h}_{k+\frac{1}{2}} \alpha_{j-k} \qquad\qquad \text{taking into account (9)}
\end{aligned}$$

and the relation (8) is a direct consequence of (6). □

3) First numerical tests

• We have compared in [DM2k] several numerical schemes *i.e.* two and three point Grünwald-Letnikov scheme, Msallam scheme and P_1 finite element scheme and we have also compared in [DM01] thoses schemes with the mixed collocation method. These tests are done for a semi-derivation, *i.e.* $\beta = 0.5$. The dynamics $(u,t) \longmapsto \Phi(u\,,t)$ is parameterized by the functions $u \longmapsto f(u)$ and $t \longmapsto g(t)$ and by the real numbers θ_f and θ_g : $\Phi(u\,,t) \;\equiv\; \theta_f\, f(u) + \theta_g\; g(t)$. The parameters θ_f and θ_g are chosen in order to obtain as solution the following particular functions :

$$u_j(t) \;\equiv\; \left(\sqrt{t}\right)^{j}\,, \qquad j = 1, \cdots, 5\,. \tag{10}$$

In a first approach, we consider $\theta_f = 0$ and $\theta_g = 1$; a simple semi-quadrature has to be done. The equation (2) corresponds to the following $t \longmapsto g(t)$ choice : $g_1(t) \;=\; \frac{1}{2}\sqrt{\pi}$, $g_2(t) \;=\; \frac{2}{\sqrt{\pi}}\sqrt{t}$, , $g_3(t) \;=\; \frac{3}{4}\sqrt{\pi}\,t$, $g_4(t) \;=\; \frac{8}{3\sqrt{\pi}}\,t\sqrt{t}$ and $g_5(t) \;=\; \frac{15}{16}\sqrt{\pi}\,t^2$.

In a second approach, we take $\theta_f \equiv 1$ and $\theta_g \equiv 0$. This dynamics is associated to the following functions :

$$(11)\qquad \begin{cases} f_1\,(u) \,=\, \dfrac{1}{2}\,\sqrt{\pi}\,, \quad f_2\,(u) \,=\, \dfrac{2}{\sqrt{\pi}}\,\sqrt{u}\,, \quad f_3\,(u) \,=\, \dfrac{3}{4}\,\sqrt{\pi}\,u^{\frac{2}{3}}\,, \\ f_4\,(u) \,=\, \dfrac{8}{3\,\sqrt{\pi}}\,u^{\frac{3}{4}}\,, \quad f_5\,(t) \,=\, \dfrac{15}{16}\,\sqrt{\pi}\,u^{\frac{4}{5}}\,. \end{cases}$$

In a third approach, whave also considered the following numerical test cases previously proposed by K. Diethelm [Di97], Diethelm and Ford [DF02], Diethelm and Luchko [DL03], Blank [Bl96] and Lubich [Lu86] :

$$(12)\qquad u \,=\, 0\,,\ t \leq 0\,, \quad D^{1/2}u \,=\, -u \,+\, \frac{8}{3\sqrt{\pi}}\,t^{\frac{3}{2}}\,, \quad t > 0\ :\ u\,(t) \,=\, t^2$$

$$(13)\qquad u \,=\, 1\,,\ t \leq 0\,, \quad D^{1/2}u \,=\, u\,, \quad t > 0\ :\ u\,(t) \,=\, e^t\,\Big(\mathrm{erf}\sqrt{t} \,+\, 1\Big)$$

$$(14)\qquad u \,=\, 1\,,\ t \leq 0\,, \quad D^{1/2}u \,=\, -u\,, \quad t > 0\ :\ u\,(t) \,=\, e^t\,\Big(1 \,-\, \mathrm{erf}\sqrt{t}\Big)$$

$$(15)\qquad u \,=\, 0\,,\ t \leq 0\,, \quad D^{1/2}u \,=\, \frac{1}{\sqrt{\pi}}\,\sin\sqrt{t}\,, \quad t > 0\,:\, u\,(t) \,=\, \sqrt{t}\,J_1\,\Big(\sqrt{t}\Big)\,.$$

• We remark that for the nonlinear cases proposed in (11), the sufficient Lipschitz continuity condition for the function $\Phi(\bullet,\bullet)$, revisited by Nagumo and presented *e.g.* the book [GV91] of Gorenflo and Vessela, that assumes that the nonlinear Abel-Volterra equation (3) has a unique continuous solution, is *a priori* not satisfied. Nevertheless, the functions presented at the relations (10) are clearly solution of problem (3) and our numerical results have captured this fact. The numerical simulation is done with our Fortran software "Semidif". We have computed systematically the orders of convergence for mesh step sizes h of the type $\frac{1}{2^n}$ for $3 \leq n \leq 13$. We have measured the L^2 and L^∞ errors denotes respectively by e_2^n and e_∞^n and defined according to : $e_\infty^n \equiv \max\{|u(jh) - u^j|, \quad j = 0, \cdots, 2^n\}$ and

$$e_2^n \equiv \sqrt{h}\sqrt{\frac{1}{2}\,|u\,(0) - u_0|^2 + \sum_{j=1}^{2^n-1}\left|u\left(\frac{j}{2^n}\right) - u_j\right|^2 + \frac{1}{2}\,|u\,(1) - u_{2n}|^2}\,.$$

The orders of convergence are summarized in the following table :

	$g_1(t)$	$g_2(t)$	$g_3(t)$	$g_4(t)$	$g_5(t)$	(12)	(13)	(14)
L^∞	∞	1.00	1.48	1.47	1.46	1.00	1.51	1.23
L^2	∞	1.40	1.47	1.46	1.45	1.00	1.50	1.42

Our results show a good agreement with the studies done by these authors. We refer to our report [DM01] for the details.

4) Nonlinear model with a singularity

• We explain in this section how to consider the $P_1 Q_0$ method when we study the Joulin model [Jo85] for spherical flammes :

$$(16) \qquad \begin{cases} D^{1/2}(u) &= \Phi\left(u\left(t\right), t\right) , \qquad t > 0 \\ u &= 0 , \qquad\qquad t \leq 0 \end{cases}$$

$$(17) \qquad \Phi\left(u\left(t\right), t\right) \;=\; \log u + \frac{E\, t^{\gamma}\, \left(1-t\right)}{u} \, \mathrm{H}(1-t) \;,$$

where E and $\gamma = 0.3$ are positive constants and $\theta \longmapsto \mathrm{H}\left(\theta\right)$ the Heaviside fonction equal to 0 if $\theta < 0$ end to 1 if $\theta > 0$.

Proposition 2. Computation of the first point for Joulin equation
For the equation (16), and the representation (8) of the unknown u^h, the first unknown point u_1^h is solution of the following equation whose unknown is denoted by x :

$$(18) \qquad x = 2\sqrt{\frac{h}{\pi}} \, \left\{ \log x - 1 + \frac{E\, h^{\gamma}}{x} \left(\frac{1}{\gamma} - \frac{h}{\gamma+1} \right) \right\} .$$

Proof of proposition 2.
We integration the equation (16) "one half" time on the interval $[0,\, h]$:

$$(19) \qquad u_1^h \;=\; \int_0^h \frac{1}{\sqrt{\pi\left(h-\theta\right)}} \, \Phi\left(u^h\left(\theta\right), \theta\right) \, \mathrm{d}\theta \, .$$

Then we make the hypothesis that the flux $\Phi\left(\bullet\, , \bullet\right)$ is equal to a constant $f_{\frac{1}{2}}^h$ on the interval $[0, h]$: $\quad f_{\frac{1}{2}}^h \;=\; \frac{1}{h}\int_0^h \Phi\left(u^h\left(\theta\right), \theta\right) \, \mathrm{d}\theta$. We inject this hypothesis at the right hand side of equation (19) :

$$(20) \qquad u_1^h \;=\; 2\sqrt{\frac{1}{\pi}} \, \frac{1}{\sqrt{h}} \, \int_0^h \Phi\left(u^h\left(\theta\right), \theta\right) \, \mathrm{d}\theta$$

and we compute the term on the right of (20) by using the function $\Phi\left(\bullet\, , \bullet\right)$ of the relation (17). We note the singularity in the vincinity of zero. The hypothesis of affine representation of u between 0 and h, show the following expression :

$$\begin{aligned} \Phi\left(u^h\left(\theta\right), \theta\right) \;&=\; \log\, \left(u_1^h \, \frac{\theta}{h} \right) \,+\, E\, \theta^{\gamma} \left(1-\theta\right) \frac{1}{u_1^h \, \frac{\theta}{h}} \qquad\qquad \text{if } h \leq 1 \\ &=\; \log\, \left(u_1^h\right) + \log\, \frac{\theta}{h} \,+\, E\, h \, \frac{\theta^{\gamma-1}\, \left(1-\theta\right)}{u_1^h} \, . \end{aligned}$$

Then after integration, we obtain

$$\begin{aligned}\int_0^h \Phi\left(u^h(\theta),\theta\right)\frac{\mathrm{d}\theta}{h} &= \log\left(u_1^h\right) + \int_0^1 \log t \,\mathrm{d}t + \frac{E}{u_1^h}\, h^\gamma \int_0^1 t^{\gamma-1}\,(1-h\,t)\,\mathrm{d}t \\ &= \log\left(u_1^h\right) + [t\,\log t - t]_0^1 + \frac{E}{u_1^h}\left[\frac{1}{\gamma} - \frac{h}{\gamma+1}\right] \\ &= \log\left(u_1^h\right) - 1 + \frac{E}{u_1^h}\left(\frac{1}{\gamma} - \frac{h}{\gamma+1}\right).\end{aligned}$$

and the proposition 2 is established. □

• The equation (18) is solved with the Newton algorithm. For the other grid points, some algebra and a numerical integration (see the details in [DM01]) show that we have to solve the system composed by (8) and the following representation :

$$f^h_{j+\frac{1}{2}} = \left\{\begin{array}{l} \dfrac{1}{u^h_{j+1} - u^h_j}\left[u^h_{j+1}\log u^h_{j+1} - u^h_{j+1}\right] - 1 \\ + \dfrac{E\,h^{\gamma-1}}{2}\left(\dfrac{j^{\gamma-1}\,(1-jh)}{u^h_j} + \dfrac{(j+1)^{\gamma-1}\,(1-(j+1)\,h)}{u^h_{j+1}}\right).\end{array}\right.$$

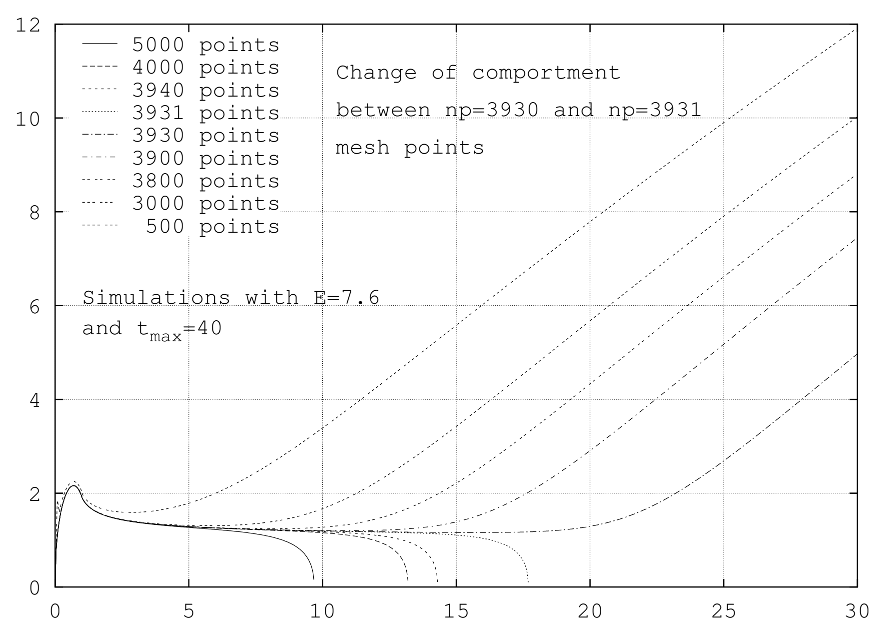

Figure 1. Qualitative change of the solution according to various discretizations.

• We have followed in [DM01] the working plan proposed by Audounet and Roquejoffre [AR98] for their simulations of the semidifferential equation (16)

(17) : $\gamma = 0.3$ and $7.6 \leq E \leq 7.7$. According to these authors, a bifurcation in the asymptotic comportment occurs for the solution of model (16)(17) with $\gamma = 0.3$. For $E \leq 7.7$, we have extinction of the flamme in a finite time whereas for $E \geq 7.8$, its radius tends to infinity as time tends to infinity.

• We first observe that we have to control very precisely the discretization step h, as proposed in the following experiment. We consider the parameter value $E = 7.6$ and $t_{\max} = 40$. When we use less than $N = 3930$ mesh points, the comportment of the discrete solution is to tends to infinity and for more than $N = 3931$ mesh points, we observe an extinction in a finite time (see the figure 1) !

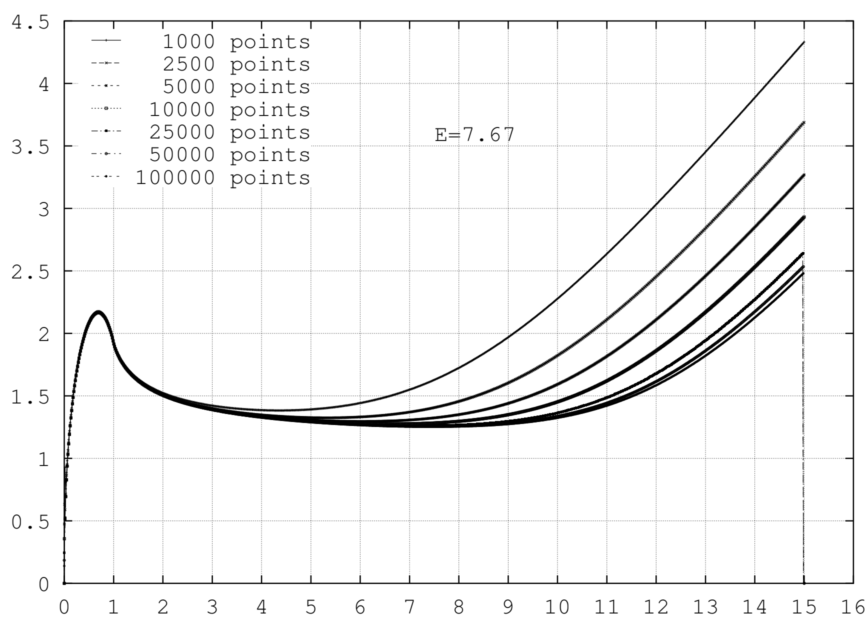

Figure 2. Numerical solution of the model (16) (17), $E = 7.67$.

• In what follows, we systematically refine the mesh in order to make in evidence the independence of the numerical solution with the number of grid points. When we use sufficiently refined meshes, we observe (see [DM01]) an extinction in finite time for $E = 7.6$ and a diverging process for $E = 7.7$. We have experimentally determined the value of bifurcation parameter E. We use a number of mesh points N according to the rule $N = \cdots, 10^k, \quad 2.5\ 10^k, \quad 5\ 10^k, \quad 10^{k+1}, \cdots$. The same conclusions hold for the extinction parameter $E = 7.66$ and we have a diverging flame for $E = 7.67$ (Figure 2), but the numerical proof needs meshes that use up to 250000 points. The case $E = 7.665$ (Figure 3) shows an extinction of the flamme in a finite time, but the high cost of computer ressources (more than two millions mesh points to observe asymptotically numerical convergence with the time discretization !) makes in evidence the actual limitations of the method. Therefore, according to our numerical results, the bifurcation parameter E for the model (16) (17) satisfies the inequalities : $7.665 < E < 7.67$ with $\gamma = 0.3$.

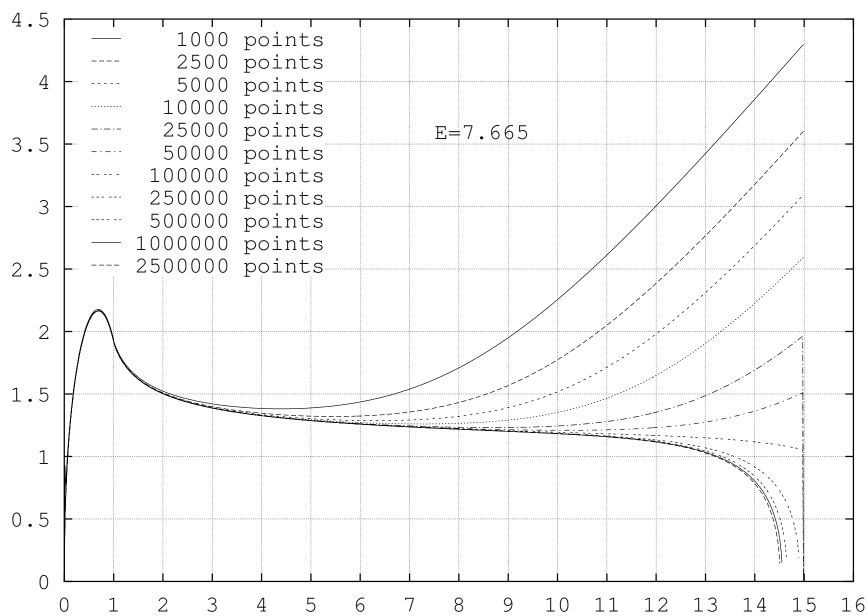

Figure 3. Numerical solution of the model (16) (17), $E = 7.665$.

5) Conclusion and aknowledgments

• In our "Semidif" software, the system of equations (7) (8) that characterizes the P^1Q^0 mixed collocation method is solved with a Newton method. We have validated our approach with exact solutions and recent published numerical approximations about fractional differential equations. For a difficult test case issued from combustion modelling, we show that our mixed collocation method is relevant and conducts to significative results. We have noticed an accuracy of order 1 for nonlinear test problems whereas the interpolation process is of order 2. The natural question is therefore to obtain second order accuracy in the future. Last but not least, we thank the unknown referee for helpful scientific comments on the first version of this article.

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