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EFFICIENCY AND ROBUSTNESS OF THE (ANDERSON-)PICARD-NEWTON ITERATION FOR SOLVING NONLINEAR PDES

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Abstract. We consider the Picard-Newton and Anderson accelerated Picard-Newton solvers applied to the Boussinesq equations, nonlinear Helmholtz equations and Liouville equation, for the purpose of accelerating convergence and improving robustness with respect to problem parameters. In all cases, we show the proposed solvers improve efficiency over the commonly used solvers and are able to find solutions for a much larger set of problem parameters.

1 INTRODUCTION

There will always be a need for faster and more robust nonlinear solvers, and in particular for nonlinear partial differential equations (PDEs). For PDEs arising from physics applications, solvers typically work well in the (easy) case when the parameters are such that the effect of the nonlinear terms is small compared to the linear terms. However, for problems such as Navier-Stokes equations (NSE) with large Reynolds number, Boussinesq equations with large Rayleigh number, Oldroyd-B with large Weissenberg number, nonlinear Helmholtz with large wave number and Kerr coefficient, and so on, nonlinear solvers can be slow or even fail when parameters

are sufficiently large. While techniques such as continuation methods can sometimes be used to "climb the ladder" up to larger parameters, such methods are typically slow, are not robust without frequent user intervention, and thus developing solvers that directly solve nonlinear PDEs with these larger parameters can provide dramatic efficiency gains and can even be an enabling technology.

Newton's method is a very widely used solver, and when it works it typically converges quadratically. In general, Newton takes the form

$$x_{k+1} = g_N(x_k) = x_k - (f'(x_k))^{-1} f(x_k),$$

where f is the function for which a root x^* is desired, $f : X \to X$ where often $X \subseteq \mathbb{R}^n$, and quadratic convergence is achieved when $g_N \in C^2$ around x^*, $g_N'(x^*) = 0$, and x_0 is sufficiently close to x^*. For nonlinear PDEs, g_N represents a solution operator to a Newton-linearized system. For most problems, a first attempt at a nonlinear solver is often to try Newton, and if it works then you are done [11]. However, Newton has a significant drawback in that it requires a good initial guess, and when it does not have a good guess it often will quickly diverge and even blow up [11, 13, 17, 19]. Moreover, in nonlinear PDEs from physics, as the important parameters increase, the size of the convergence basin for both initial guesses and problem parameters decreases.

An alternative to Newton that typically has less restrictions on the initial guess (i.e. has a larger convergence basin than Newton) is the Picard iteration, which takes the form

$$x_{k+1} = g_P(x_k),$$

and often (for a carefully designed Picard iteration)

$$\|g_P'\| \leq \alpha < 1$$

in an appropriate norm, in some region containing x^*. For nonlinear PDEs, g_P typically represents a solution operator to a (Picard-) linearized system. The Picard iteration converges linearly under this assumption, and other nice properties of Picard are that it often has better stability properties than Newton, and for coupled problems is generally more efficient since it can allow for more stable decoupling of the system in the linear solve. Unfortunately, convergence of Picard is slow, often just linear, and the rate gets worse as the important PDE parameters increase - and then once the parameters are large enough, it fails. It is shown in [18, 8, 16] how Anderson acceleration (AA) can improve the convergence properties of Picard in many cases. It was also shown in [21] how AA often decreases the convergence rate of Newton (in general, although it can help when the Jacobian is close to singular [5, 6] or Newton converges linearly or does not converge at all).

In the recent paper [17], the Picard-Newton (PN) and Anderson accelerated Picard-Newton (AAPN) iterations were proposed as solvers for the NSE. While various combinations of Picard and Newton have been considered over the years [22, 14, 20, 15], the paper [17] showed that a direct composition of these solvers, i.e.

$$g_{PN} = g_N \circ g_P,$$

were remarkably effective for the NSE and allowed convergence for much higher Reynolds number than Picard or Newton on their own. We note that composition of nonlinear solvers in general has recently been found to be an effective strategy [4], and can combine the good properties of the solvers being combined; in the case of Picard-Newton, the aim is to combine the speed of Newton with the robustness and stability of Picard. Mathematical theory was also developed in [17] that showed for the NSE the proposed Picard-Newton and AA-Picard-Newton algorithms had better stability and convergence properties than Picard or Newton individually.

For simplicity, for AA we will consider only depth $m = 1$ AA applied to Picard, and without relaxation. This takes the form: Given x_k,

Step 1. Find $\tilde{x}_{k+1} = g(x_k)$.

Step 2. Find $\hat{x}_{k+1} = g(\tilde{x}_{k+1})$.

Step 3. Find α_{k+1} satisfying

$$\alpha_{k+1} = \text{argmin}_\alpha \|\alpha(\hat{x}_{k+1} - \tilde{x}_{k+1}) + (1-\alpha)(\tilde{x}_{k+1} - x_k)\|.$$

Step 4: Set $x_{k+1} = \alpha_{k+1}\hat{x}_{k+1} + (1-\alpha_{k+1})\tilde{x}_{k+1}$.

We note that AA applied to g_P can itself be considered a fixed point iteration, and we denote it as g_{AAP}. As proven in [12], since g_P is assumed contractive in a region around x^*, g_{AAP} is contractive in a region that is at least almost as big (and asymptotically at least as big). In practice, the contractive region is usually significantly bigger for g_{AAP} compared to g_P, [16], however, theory to classify this remains an open problem.

The purpose of this paper is to extend the ideas of [17] beyond the NSE. To give the reader some intuition for why (AA-)Picard-Newton works, consider the simple case of real-valued functions with the Picard-Newton iteration g_{PN}, where $x^* \in \Omega$,

$$g_N(x^*) = g_P(x^*) = 0$$

with $g_N \in C^2(\Omega)$, $g_P \in C^2(\Omega)$, $g_N'(x^*) = 0$ and $\|g_P'\| \leq \alpha < 1$ on Ω. A straightforward calculation using the chain rule shows that for $x \in \Omega$,

$$g_{PN}'(x) = g_N'(g_P(x)) \cdot g_P'(x),$$

and thus for $x = x^*$,

$$g_{PN}'(x^*) = g_N'(g_P(x^*)) \cdot g_P'(x^*) = g_N'(x^*) \cdot g_P'(x^*) = 0, \tag{1}$$

and additionally

$$\|g_{PN}'(x)\| = \|g_N'(g_P(x)) \cdot g_P'(x)\| = \|g_N'(g_P(x))\|\|g_P'(x)\| \leq \alpha \|g_N'(g_P(x))\|. \tag{2}$$

From (1) we observe that Picard-Newton is quadratically convergent. From (2), in the region where $\|g'_N\|$ is a monotonically increasing function of $(x - x^*)$ (which is at least an interval around x^* with positive radius), then since $x \in \Omega$ we can infer that $\|g'_{PN}(x)\| \leq \alpha \|g'_N(x)\|$. Since $\alpha < 1$, this suggests that Picard-Newton will have a larger contractive region than Newton, which is exactly what we observed for Picard-Newton applied to NSE in [17].

This simplified analysis above gives results very similar to what was found with a much more technical analysis for the Picard-Newton iteration for the NSE. Hence it is reasonable to conjecture that we will see similar behavior for Picard-Newton applied to other types of nonlinear PDEs. We consider herein the Picard-Newton and AA-Picard-Newton solvers to the nonlinear Helmholtz equation, Liouville equation, and Boussinesq system, which show the proposed methods are very effective nonlinear solvers that can improve both efficiency and robustness compared to Picard and Newton.

2 APPLICATION 1: NONLINEAR HELMHOLTZ EQUATION

We consider as a first application the nonlinear Helmholtz equation from optics, where the interest is in the propagation of continuous-wave laser beams through transparent dielectrics. The system we consider is taken from [1] and takes the following form: Find $u : [0, 10] \to \mathbb{C}$ satisfying

$$\begin{aligned} \frac{d^2u}{dx^2} + k^2(1 + \epsilon(x)|u|^2)u = 0, \quad & 0 < x < 10 \\ \frac{du}{dx} + iku = 2ik, \quad & x = 0, \\ \frac{du}{dx} - iku = 0, \quad & x = 10, \end{aligned} \tag{3}$$

where u represents the unknown complex scalar electric field, k is the linear wavenumber, $\epsilon(x)$ is a material dependent quantity depending on the linear index of refraction and Kerr coefficient, and the boundary conditions are known as two-way boundary conditions that allows waves to enter and exit the domain in a physically consistent manner [9]. Despite being 1D, this system is well known to be quite challenging due to the cubic nonlinearity, especially as ϵ and k get larger. Solutions for $k = 5,\ \epsilon = 0.1$ and $k = 10,\ \epsilon = 0.3$ are shown in figure 1, and we observe a more complex behavior as the parameters increase.

We test here the Picard, Newton, Picard-Newton, and AA-Picard-Newton iterations for the nonlinear Helmholtz equation. The Picard iteration takes the form

$$\begin{aligned} (u_{j+1})_{xx} + k^2 u_{j+1} + k^2 \epsilon(x)|u_j|^2 u_{j+1} = 0, \quad & 0 < x < 10, \\ (u_{j+1})_x + iku_{j+1} = 2ik, \quad & x = 0, \\ (u_{j+1})_x - iku_{j+1} = 0, \quad & x = 10, \end{aligned}$$

and the Newton iteration is similar to Picard except that the nonlinear term is instead

$$k^2\epsilon(x)\left((u_j^* u_j)u_{j+1} + (u_{j+1}^* u_j)u_j + (u_j^* u_{j+1})u_j - 2(u_j^* u_j)u_j\right).$$

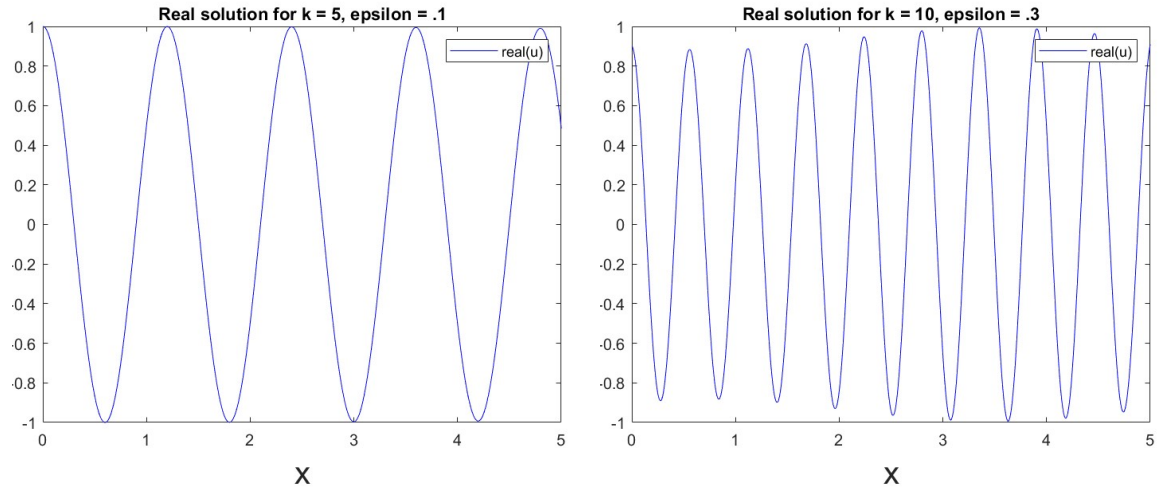

Figure 1: Shown above are solutions (real part only) for nonlinear Helmholtz problem with varying ϵ and k

We discretize the linearized systems in space with a second order finite difference approximation using N equally spaced points (we tested 1001, 2001 and 4001, and observed very similar results for each, and so results below are only for $N = 4001$), and for an initial guess we use the nodal interpolant of

$$u_0 = (\cos(kx) + i\sin(kx)),$$

i.e. the linear ($\epsilon = 0$) Helmholtz equation solution for a given k.

Our objective centers around achieving convergence specifically for larger values of k and ϵ. Table 1 shows the number of iterations needed for Picard, Newton, Picard-Newton and AA-Picard-Newton iterations to achieve convergence for $k = 5$ and varying values of ϵ. Newton iteration converges up to a value of $\epsilon = 0.12$, Picard iteration has a slightly better behavior, achieving convergence for ϵ values up to 0.23. We observe that both Picard-Newton and AA-Picard-Newton iterations converge up to an ϵ value of 0.45, and in most cases AA-Picard-Newton converges faster.

Shown in table 2 are results for $k = 20$ and varying ϵ, as number of iterations needed to converge for Picard, Newton, Picard-Newton and AA-Picard-Newton. We observe that Picard iteration achieves convergence up to an ϵ of 0.07, whereas Newton iteration only converges for smaller ϵ values (up to 0.03). AA-Picard-Newton and Picard-Newton show notable improvements in comparison to Picard and Newton iterations. AA-Picard-Newton achieves convergence for ϵ values up to 0.14, while Picard-Newton achieves convergence for slightly higher ϵ values (up to 0.18).

3 APPLICATION 2: BOUSSINESQ EQUATIONS

For our next application problem, we consider the Boussinesq equations, which describe non-isothermal flow. Typically such are flows driven by buoyancy in applications such as ven-

Table 1: Shown below are the number of iterations needed for convergence with $k = 5$, $N = 4001$ and varying ϵ for the nonlinear Helmholtz problem, using a tolerance of 10^{-8} in the l^2 norm. .

ϵ	Picard	Newton	PN	AAPN
0.01	8	4	3	3
0.03	11	5	3	3
0.06	16	6	4	3
0.09	19	7	4	3
0.12	29	8	4	4
0.15	46	F	5	4
0.18	59	F	5	4
0.21	61	F	6	5
0.23	237	F	7	5
0.24	F	F	8	5
0.27	F	F	231	7
0.3	F	F	607	34
0.33	F	F	248	11
0.36	F	F	20	33
0.39	F	F	733	200
0.42	F	F	F	285
0.45	F	F	157	15
0.48	F	F	F	F

Table 2: Shown below are the number of iterations needed for convergence with $k = 20$, $N = 4001$ and varying ϵ for the nonlinear Helmholtz problem, using a tolerance of 10^{-8} in the l^2 norm.

ϵ	Picard	Newton	PN	AAPN
0.01	12	5	3	3
0.03	21	8	4	3
0.04	34	F	4	4
0.06	89	F	5	4
0.07	160	F	5	5
0.08	F	F	6	5
0.09	F	F	7	5
0.12	F	F	51	445
0.14	F	F	132	409
0.15	F	F	251	F
0.18	F	F	1871	F
0.21	F	F	F	F

tilation, solar collectors, and window insulation. The steady Boussinesq system takes the form,

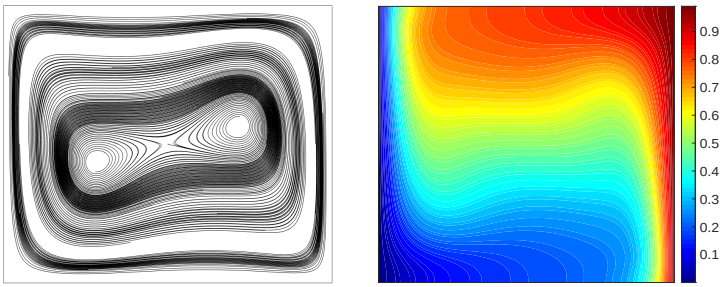

Figure 2: The $Ra = 10^5$ Boussinesq velocity (left) and temperature (right) solutions are shown above for the differentially heated cavity problem.

let $\Omega \subset \mathbb{R}^d$ (d=2 or 3):

$$\begin{aligned} u \cdot \nabla u - \nu \Delta u + \nabla p &= Ri\langle 0, \theta \rangle^T + f, \\ \nabla \cdot u &= 0, \\ u \cdot \nabla \theta - \kappa \Delta \theta &= \gamma, \end{aligned} \tag{4}$$

with u representing the velocity, p the pressure, θ the temperature (or density), and f and γ the external momentum forcing and thermal sources. The kinematic viscosity $\nu > 0$ is defined as the inverse of the Reynolds number ($Re = \nu^{-1}$), and the thermal conductivity $\kappa = Re^{-1}Pr^{-1}$ where Pr is the Prandtl number and Ri is the Richardson number. Appropriate boundary conditions are required to determine the system. The Rayleigh number is defined by

$$Ra = Ri \cdot Re^2 \cdot Pr,$$

and higher Ra leads to more complex physics as well as more difficulties in numerically solving the system.

The Newton iteration for the Boussinesq system takes the form

$$u_k \cdot \nabla u_{k+1} + u_{k+1} \cdot \nabla u_k - u_k \cdot \nabla u_k - \nu \Delta u_{k+1} + \nabla p_{k+1} = Ri\langle 0, \theta_{k+1} \rangle^T + f, \tag{5}$$

$$\nabla \cdot u_{k+1} = 0, \tag{6}$$

$$u_k \cdot \nabla \theta_{k+1} + u_{k+1} \cdot \nabla \theta_k - u_k \cdot \nabla \theta_k - \kappa \Delta \theta_{k+1} = \gamma, \tag{7}$$

together with appropriate boundary conditions.

The Picard iteration for Boussinesq takes the form

$$u_k \cdot \nabla u_{k+1} - \nu \Delta u_{k+1} + \nabla p_{k+1} = Ri\langle 0, \theta_{k+1} \rangle^T + f, \tag{8}$$

$$\nabla \cdot u_{k+1} = 0, \tag{9}$$

$$u_k \cdot \nabla \theta_{k+1} - \kappa \Delta \theta_{k+1} = \gamma. \tag{10}$$

We note that the Picard iteration will decouple into a temperature equation which is solved first and then an Oseen type solve is done to recover the next velocity and pressure. Effective preconditioners for these systems exist in the literature [2, 7, 10, 3].

We consider the test problem often called the 'differentially heated cavity', which models internal flow in a square cavity where horizontallly opposite walls have different fixed temperatures, and the top and bottom are insulated. We take $\Omega = (0,1)^2$, no forcing of the momentum or temperature $f = 0, \gamma = 0$, no slip velocity boundary conditions on all sides, perfect insulation on the top and bottom $\nabla T \cdot n = 0$ where n is the outward unit normal, $T = 1$ on the right side and $T = 0$ on the left. The solution for $Ra = 10^5$ is shown in figure 2.

We discretize using a barycenter refinement of a $\frac{1}{64}$ uniform triangular mesh, using (P_2, P_1^{disc}) Scott-Vogelius elements for the velocity and pressure, and P_2 elements for temperature. The Dirichlet boundary conditions are enforced strongly, and the perfect insulation condition is enforced weakly with a do-nothing condition.

We test the Picard, Newton, Picard-Newton and AAPicard-Newton solvers for this system, for varying Ra. Results are shown in table 3, and we observe that both Newton and Picard iterations converge up to Ra =10000 but fail at Ra=25000 and above. When Newton fails, the residual grew very large, while for Picard the iterations remained stable even though convergence was not reached in 200 iterations. A major improvement in seen from using Picard-Newton, as here convergence is achieved up to Ra =250000, well over an order of magnitude better than Picard and Newton on their own, and up to Ra =100000 the quadratic convergence of Picard-Newton is observed. AA-Picard-Newton has slightly better convergence behavior than Picard-Newton in that it can converge up to Ra =500000, and for moderate Ra AA-Picard-Newton converges in fewer iterations (for small Ra they converge in the same number of iterations).

Table 3: Shown below are the number of iterations needed for residual convergence for the heated cavity problem with varying Rayleight number Ra for the Boussinesq problem, using a tolerance of 10^{-8} in the $H^1 \times H^1$ norm for velocity and temperature. An F indicated the residual grew to above 10^5, and DNC indicates no convergence in 200 iterations.

Ra	Picard	Newton	PN	AAPN
1000	12	6	5	5
5000	55	8	6	6
10000	144	9	7	8
25000	DNC	F	9	8
50000	DNC	F	13	10
100000	DNC	F	16	11
250000	DNC	F	159	16
500000	DNC	F	DNC	93
1000000	DNC	F	DNC	DNC

4 APPLICATION 3: LIOUVILLE EQUATION

For our final application we consider the Liouville equation which arises in fluid mechanics. We consider it in the following form on $\Omega \subset \mathbb{R}^d$ by

$$\begin{aligned} \Delta u + e^{\lambda u} &= 0, \\ u|_{\partial\Omega} &= 0, \end{aligned}$$

and our tests use $d = 2$. A solution on $\Omega = (0, 1)^2$ and $\lambda = 5$ is shown in figure 3. The goal for the solvers is to get solutions for λ as large as possible.

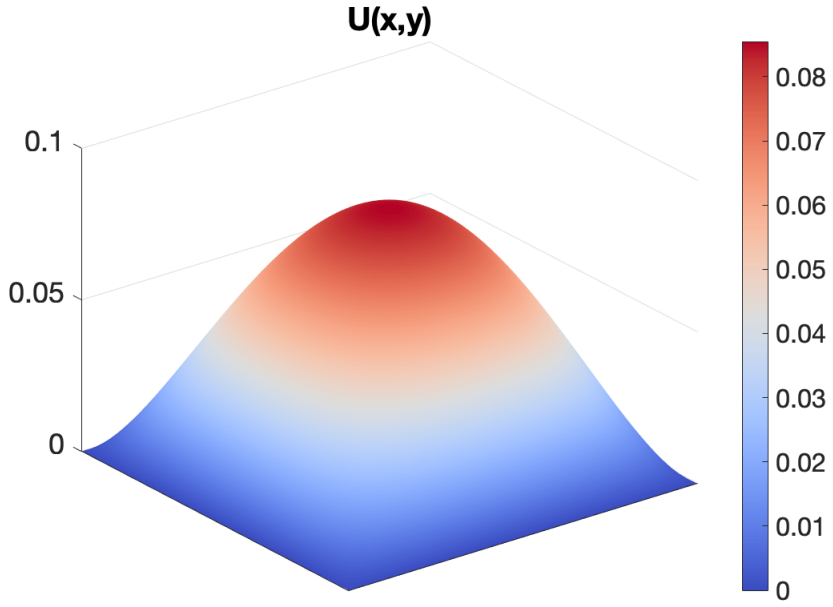

Figure 3: Shown above is a solution for Liouville equation with $\lambda = 5$.

The Picard iteration for this system is defined by lagging the unknown in the exponential via

$$\begin{aligned} -\Delta u_{k+1} &= e^{\lambda u_k} \\ u_{k+1}|_{\partial\Omega} &= 0. \end{aligned}$$

The Newton iteration is derived from defining

$$F(v) = \Delta v + e^{\lambda v}$$

and then calculating using

$$u_{k+1} = u_k - F'(u_k)^{-1}[F(u_k)]$$

to get the iteration

$$-\Delta u_{k+1} - \lambda e^{\lambda u_k} u_{k+1} = -\lambda u_k e^{\lambda u_k} + e^{\lambda u_k}.$$

These iterations are solved using the finite element method with continuous P_2 elements on a uniform triangular $h = \frac{1}{64}$ mesh (although we note we ran the tests for different h and obtained very similar results). The initial condition for our tests is $u_0 = 0$.

Results for the solvers are shown in table 4 for Picard, Newton, Picard-Newton and AA-Picard-Newton, as well as AA applied to the Picard-Newton iteration itself (AAPicard-Newton only applied AA to the Picard iteration step). We observe that Newton does slightly better than Picard, and converges up to $\lambda = 7$ whereas Picard converges only up to $\lambda = 6$. Picard-Newton also only converges up to 7 as does AA-Picard-Newton, although they need less iterations to converge compared to Newton. AA applied to (Picard-Newton) performs the best for this test, and is able to get solutions up to $\lambda = 11$.

Table 4: Shown below are iterations needed to converge solvers for the Liouville problem to 10^{-8} in the L^2 norm of the residual. An F indicates that the residual grew to bigger than 10^5.

λ	Picard	Newton	PN	APPN	AAPN
1	7	4	3	3	2
2	9	5	4	3	3
3	11	6	5	3	3
4	13	8	6	4	3
5	18	11	8	4	4
6	27	18	12	6	4
7	F	41	24	16	5
8	F	F	F	F	7
9	F	F	F	F	11
10	F	F	F	F	17
11	F	F	F	F	41
12	F	F	F	F	F

5 CONCLUSIONS

We extended the Picard-Newton and AA-Picard-Newton solver methodology to three new tests problems: nonlinear Helmholtz, Boussinesq and Liouville equations. In all cases we observe improvement from the composition of Picard and Newton (and with AA) over both Picard and Newton, allowing for convergence for a wider range of physical parameters. The amount of improvement varies across the test problems, with modest improvement for Liouville, significant improvement for nonlinear Helmholtz, and remarkable improvement for Boussinesq. Future work includes developing convergence analsysis for Picard-Newton and AA-Picard-Newton for these systems as well as a general theory.

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