

# The Stiff Limit of the Exponential Rosenbrock-Type Method

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# Stiff Decay

- An system is considered 'stiff' if the ODE contains multiple time scales, with both rapidly oscillating modes and slow dynamics.
- After enough time has passed, a larger step size is sufficient to accurately capture the behavior of the system.
- To determine whether a problem has stiff decay, we consider the eigenvalues of the Jacobian from the equation of motion.
- Problems exhibiting stiff decay can have
  - a mixture of eigenvalues with large, negative real parts and eigenvalues with small negative real parts, or
  - eigenvalues that are large and almost purely imaginary.

# The Exponential Rosenbrock-type Method

- The first prototypes of exponential integrators have existed for nearly 50 years.
- Historically, most exponential-style integrators linearized the equation at the initial time step only.
- Recently, people began to linearize the problem with each time step, resulting in a much more accurate solution curve.

- The exponential Rosenbrock-type integrator is an explicit one-step method.
- With each step, the method linearizes the equation, using a Taylor expansion.

$$\begin{aligned}\mathbf{y}' &= f(\mathbf{y}) \\ &\approx f(\mathbf{y}_{k-1}) + \left. \frac{df}{d\mathbf{y}} \right|_{\mathbf{y}=\mathbf{y}_{k-1}} (\mathbf{y} - \mathbf{y}_{k-1}) \\ &= f(\mathbf{y}_{k-1}) + J(\mathbf{y} - \mathbf{y}_{k-1})\end{aligned}$$

- Using the matrix exponential, the exponential Rosenbrock-type integrator solves the linear equation exactly, then steps forward by the exact solution of the linear equation.

- The solution to the linear equation is

$$\mathbf{y}_k = e^{(t-t_{k-1})J} \mathbf{y}_{k-1} + \int_{t_{k-1}}^{t_k} e^{(t_k-\tau)J} d\tau (f(\mathbf{y}_{k-1}) - J\mathbf{y}_{k-1})$$

- Assuming the inverse Jacobian exists, one can use  $J^{-1}$  to calculate the integral of the matrix exponential, and for  $h = t - t_{k-1}$ , the equation becomes

$$\begin{aligned} \mathbf{y}(t) &= e^{hJ} \mathbf{y}_{k-1} + (e^{hJ} - I) J^{-1} (f(\mathbf{y}_{k-1}) - J\mathbf{y}_{k-1}) \\ &= e^{hJ} \mathbf{y}_{k-1} + (e^{hJ} - I) J^{-1} f(\mathbf{y}_{k-1}) - (e^{hJ} - I) \mathbf{y}_{k-1} \end{aligned}$$

## The Exponential Rosenbrock-Type Method

$$\mathbf{y}(t) = \mathbf{y}_{k-1} + (e^{hJ} - I) J^{-1} f(\mathbf{y}_{k-1})$$

# Standard Methods to Test Stiff Decay

- Consider testing the exponential Rosenbrock-type method with the autonomous ‘test’ equation  $\mathbf{y}' = \lambda \mathbf{y}$ .
- For  $z = h\lambda$ , we obtain  $\mathbf{y}_k = e^z \mathbf{y}_{k-1}$ , so the method solves the linear autonomous equation exactly.
- Hence, Ascher and Petzold’s approach to determining stiff decay is useless here, since the stiff decay property for the linear autonomous equation is trivial.
- Instead, we test the method on systems with stiff decay.
- To achieve stiff decay, we use test equations containing both fast and slow modes.

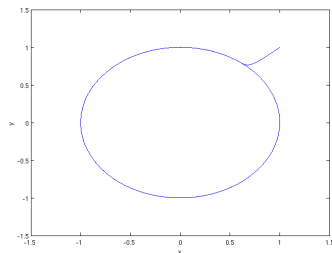
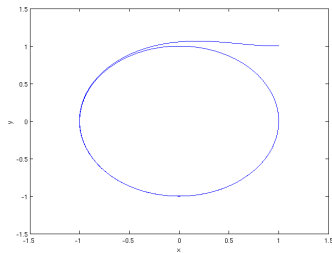
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- Instead, we test the method on systems with stiff decay.
- To achieve stiff decay, we use test equations containing both fast and slow modes.

- For the first test equation, consider a particle with some initial position.

$$\begin{cases} \dot{x} = -y - \lambda x(x^2 + y^2 - 1) \\ \dot{y} = x - \lambda y(x^2 + y^2 - 1) \end{cases}$$

- The decay to the circle provides the fast mode, then counter-clockwise rotation acts as the slow mode.
- Higher values of  $\lambda$  correspond with stiffer decay
  - Top figure:  $\lambda = 1$ , bottom figure:  $\lambda = 20$

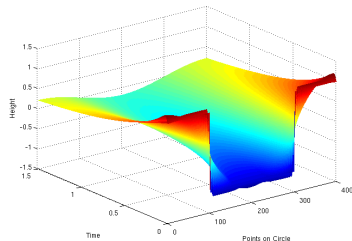
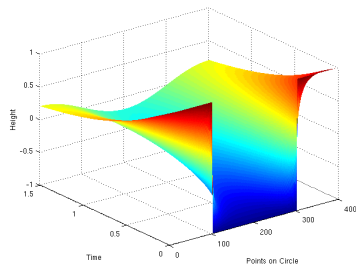


- For the second test equation, consider points a circle with diffusion or hyperviscosity and nonlinear forcing:

$$u_t = u_{xx} - u^3$$

$$u_t = u_{xxxx} - u^3$$

- Finite differences are used for the derivative in  $x$ .
- A larger number of points corresponds with greater stiffness.
- Figures show 400 points,  $t = 1.5$ .



## Properties of a Method Exhibiting Stiff Decay

- If the method properly handles stiff decay, it will traverse the slow dynamics with a step size that is not small.
- The exponential Rosenbrock-type method allows the fast modes to continue to decay as the system travels through the slow dynamics.
- Once the system has passed through the region of rapid decay, the step size  $h$  should be prescribed by the slow dynamics of the system.
- Ideally, the step size depends on the tolerance level set for the solver, and is not based on the stiffness of the problem.

# Analysis of Step Size Choice

- We apply the exponential Rosenbrock-type method to the equation  $\mathbf{y}' = \lambda \mathbf{F} + \mathbf{f} = \mathcal{F}$ 
  - $\mathbf{F}$  denotes the fast decaying modes of the system.
  - $\mathbf{f}$  denotes the slow modes of the system.
  - By assumption,  $\mathbf{f}$  is not large in  $\lambda$ .
- Then for the Jacobian we have  $\lambda \mathbf{J} + \mathbf{j} = \mathcal{J}$

- For simplicity, consider the method beginning at time 0 with a step size of  $h$ .
- Apply one step of  $h$  to obtain  $\mathbf{y}_k$  and two steps of  $h/2$  to obtain  $\bar{\mathbf{y}}_k$ .

$$\mathbf{y}_k = \mathbf{y}_{k-1} + \int_0^h e^{\tau \mathcal{J}_{k-1}} \mathcal{F}_{k-1} d\tau$$

$$\mathbf{y}_{k-1/2} = \mathbf{y}_{k-1} + \int_0^{h/2} e^{\tau \mathcal{J}_{k-1}} \mathcal{F}_{k-1} d\tau$$

$$\bar{\mathbf{y}}_k = \mathbf{y}_{k-1/2} + \int_0^{h/2} e^{\tau \mathcal{J}_{k-1/2}} \mathcal{F}_{k-1/2} d\tau$$

Let  $\mathcal{J} \triangleq \mathcal{J}_{k-1}$ ,  $\mathcal{F} \triangleq \mathcal{F}_{k-1}$ ,  $\tilde{\mathcal{J}} \triangleq \mathcal{J}_{k-1/2}$ , and  $\tilde{\mathcal{F}} \triangleq \mathcal{F}_{k-1/2}$ .

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$$\mathbf{y}_k = \mathbf{y}_{k-1} + \int_0^h e^{\tau \mathcal{J}} \mathcal{F} d\tau$$

$$\begin{aligned} \mathbf{y}_{k-1/2} &= \mathbf{y}_{k-1} + \int_0^{h/2} e^{\tau \mathcal{J}} \mathcal{F} d\tau \\ \bar{\mathbf{y}}_k &= \mathbf{y}_{k-1/2} + \int_0^{h/2} e^{\tau \tilde{\mathcal{J}}} \tilde{\mathcal{F}} d\tau \end{aligned}$$

Let  $\mathcal{J} \triangleq \mathcal{J}_{k-1}$ ,  $\mathcal{F} \triangleq \mathcal{F}_{k-1}$ ,  $\tilde{\mathcal{J}} \triangleq \mathcal{J}_{k-1/2}$ , and  $\tilde{\mathcal{F}} \triangleq \mathcal{F}_{k-1/2}$ .

- Then subtracting the two methods yields equation (4).

$$\mathbf{y}_k - \bar{\mathbf{y}}_k = \left[ \mathbf{y}_{k-1} + \left( \int_0^h e^{\tau \mathcal{J}} d\tau \right) \mathcal{F} \right] - \left[ \mathbf{y}_{k-1} + \left( \int_0^{h/2} e^{\tau \mathcal{J}} d\tau \right) \mathcal{F} + \left( \int_0^{h/2} e^{\tau \tilde{\mathcal{J}}} d\tau \right) \tilde{\mathcal{F}} \right]$$

- One can split the first integral into two pieces,  $\int_0^{h/2} e^{\tau \mathcal{J}} d\tau$  and  $\int_{h/2}^h e^{\tau \mathcal{J}} d\tau$ .

- Consider the Taylor expansion of  $\tilde{\mathcal{F}}$ , where the ellipses represent the nonlinear terms.

$$\begin{aligned}\tilde{\mathcal{F}} &= \mathcal{F} + \mathcal{I} \left( \int_0^{h/2} e^{\tau \mathcal{I}} \right) \mathcal{F} + \dots \\ &= \left[ I + \mathcal{I} \left( \int_0^{h/2} e^{\tau \mathcal{I}} \right) \right] \mathcal{F} + \dots\end{aligned}$$

- One can show that that  $I + \mathcal{I} \left( \int_0^{h/2} e^{\tau \mathcal{I}} \right) = e^{\frac{h}{2} \mathcal{I}}$ .
- Using this identity and solving for the nonlinear terms allows the expression for  $\tilde{\mathcal{F}}$  to be rewritten as

$$\tilde{\mathcal{F}} = e^{\frac{h}{2} \mathcal{I}} \mathcal{F} + (\tilde{\mathcal{F}} - e^{\frac{h}{2} \mathcal{I}} \mathcal{F})$$

- Finally, the method bounds the difference  $|\mathbf{y} - \bar{\mathbf{y}}|$  by the tolerance level, TOL.

$$|\mathbf{y} - \bar{\mathbf{y}}| = \left| \left[ \int_0^{h/2} (e^{\tau \mathcal{J}} - e^{\tau \tilde{\mathcal{J}}}) d\tau \right] e^{\frac{h}{2} \mathcal{J}} \mathcal{F} + \left[ \int_0^{h/2} e^{\tau \tilde{\mathcal{J}}} d\tau \right] (e^{\frac{h}{2} \mathcal{J}} \mathcal{F} - \tilde{\mathcal{F}}) \right| \leq \text{TOL}$$

- There are two main sources of difference between the methods used to obtain  $\mathbf{y}$  and  $\bar{\mathbf{y}}$ : the difference in the exponential terms due to rotation of the Jacobian matrix, and the nonlinear terms of the expansion for  $\tilde{\mathcal{F}}$ .

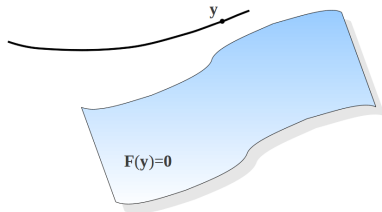
$$|\mathbf{y} - \bar{\mathbf{y}}| = \left| \left[ \int_0^{h/2} (e^{\tau \mathcal{J}} - e^{\tau \tilde{\mathcal{J}}}) d\tau \right] e^{\frac{h}{2} \mathcal{J}} \mathcal{F} + \left[ \int_0^{h/2} e^{\tau \tilde{\mathcal{J}}} d\tau \right] (e^{\frac{h}{2} \mathcal{J}} \mathcal{F} - \tilde{\mathcal{F}}) \right| \leq \text{TOL}$$

- In the linear case,  $\tilde{\mathcal{F}}$  exactly equals  $e^{\frac{h}{2} \mathcal{J}} \mathcal{F}$ .
- For the purposes of this analysis, we assume the nonlinear terms in the expansion are small, so the second term of the expression can be neglected.
- Then the difference becomes

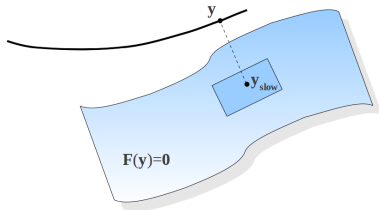
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# Analysis of Decay to the Stable Manifold

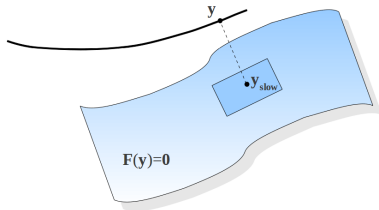
- Consider the equation  $\mathbf{y}' = \lambda \mathbf{F}(\mathbf{y}) + \mathbf{f}(\mathbf{y}) \triangleq \mathcal{F}(\mathbf{y})$ .
- We use estimation style analysis to evaluate behavior in the stiff limit ( $\lambda \rightarrow \infty$ ).
- With a large value of  $\lambda$ , we expect fast decay to the stable manifold  $\mathbf{F}(\mathbf{y}) = \mathbf{0}$ .
- Let the dimension of this surface be  $m$ , while the dimension of the whole space  $\mathbf{y}$  is  $M$ .



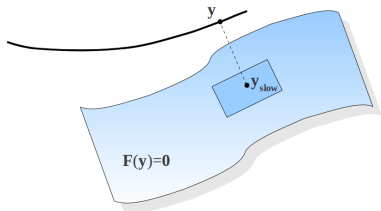
- Write  $\mathbf{y}$  as  $\mathbf{y} = \mathbf{y}_{\text{fast}} + \mathbf{y}_{\text{slow}}$ , where  $\mathbf{y}_{\text{fast}}$  corresponds to the fast decay part of the evolution, while  $\mathbf{y}_{\text{slow}}$  represents the slow evolution of the system after the decay occurs.
- Of course,  $\mathbf{y}' = (\mathbf{y}_{\text{fast}} + \mathbf{y}_{\text{slow}})' = \mathcal{F}(\mathbf{y}_{\text{fast}} + \mathbf{y}_{\text{slow}})$ .
- But this yields only  $M$  equations for  $2M$  variables.

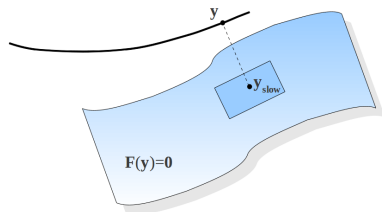


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- Choose the other  $M$  conditions according to the intuitive meaning of  $\mathbf{y}_{\text{fast}}$  and  $\mathbf{y}_{\text{slow}}$ .
- Since the manifold contains the slow dynamics,  $\mathbf{F}(\mathbf{y}_{\text{slow}}) = \mathbf{0}$ . ( $M - m$  conditions)
- Consider distributing  $\mathbf{y}$  into  $\mathbf{y}_{\text{fast}}$  and  $\mathbf{y}_{\text{slow}}$ .
- One way is to choose  $\mathbf{y}_{\text{slow}}$  as the closest point on the surface  $\mathbf{F}(\mathbf{y}) = \mathbf{0}$ . This defines an “algorithm” of finding  $\mathbf{y}_{\text{fast}}$  and  $\mathbf{y}_{\text{slow}}$  given  $\mathbf{y}$ . ( $m$  conditions)





- Consider a point  $\mathbf{y}_{slow}$  on the surface  $\mathbf{F}(\mathbf{y}) = \mathbf{0}$ .
- Let  $\hat{P}_{slow}$  be the orthogonal projector matrix to the tangent plane at  $\mathbf{y}_{slow}$ .
- Denote the complimentary projector as  $\hat{P}_{fast}$ .
- The remaining conditions now are written as  $\hat{P}_{slow} \mathbf{y}_{fast} = \mathbf{0}$ .
- This yields  $m$  additional conditions because only  $m$  singular values of  $\hat{P}_{slow}$  are non-zero.

- Let  $\hat{J} = \frac{\partial \mathbf{F}}{\partial \mathbf{y}}$ .
- The structure of  $\hat{J}$  determines the projectors  $\hat{P}_{\text{slow}}$  and  $\hat{P}_{\text{fast}} = \hat{I} - \hat{P}_{\text{slow}}$ .
- The system of equations is the following:

$$\begin{aligned}
 (\mathbf{y}_{\text{fast}} + \mathbf{y}_{\text{slow}})' &= \lambda \mathbf{F}(\mathbf{y}_{\text{fast}} + \mathbf{y}_{\text{slow}}) + \mathbf{f}(\mathbf{y}_{\text{fast}} + \mathbf{y}_{\text{slow}}); \\
 \mathbf{F}(\mathbf{y}_{\text{slow}}) = \mathbf{0}, \quad \Rightarrow \quad \hat{J}(\mathbf{y}_{\text{slow}}) \mathbf{y}'_{\text{slow}} &= \mathbf{0} \quad \text{or} \quad \hat{P}_{\text{fast}} \mathbf{y}'_{\text{slow}} = \mathbf{0}; \\
 \hat{P}_{\text{slow}} \mathbf{y}_{\text{fast}} &= \mathbf{0}.
 \end{aligned}$$

- We can then use adiabatic approximation on the system. Here we just show the leading order.
- We expect  $\mathbf{y}_{\text{fast}} \sim 1/\lambda$ , so expanding about  $\mathbf{y}_{\text{slow}}$ ,  
 $\mathbf{F}(\mathbf{y}) = (\mathbf{F}(\mathbf{y}_{\text{slow}}) = \mathbf{0}) + \hat{\mathbf{J}}(\mathbf{y}_{\text{slow}})\mathbf{y}_{\text{fast}} + \mathcal{O}(1/\lambda^2)$ .
- Consider  $(\mathbf{y}_{\text{fast}} + \mathbf{y}_{\text{slow}})' = \lambda\mathbf{F}(\mathbf{y}_{\text{fast}} + \mathbf{y}_{\text{slow}}) + \mathbf{f}(\mathbf{y}_{\text{fast}} + \mathbf{y}_{\text{slow}})$ .  
 The leading order is

$$\mathbf{y}'_{\text{slow}} = \lambda\hat{\mathbf{J}}(\mathbf{y}_{\text{slow}})\mathbf{y}_{\text{fast}} + \mathbf{f}(\mathbf{y}_{\text{slow}})$$

- Acting on the system with the fast projector,  $\hat{\mathbf{P}}_{\text{fast}}$ , projects the system onto the region of fast decay:

$$\lambda\hat{\mathbf{P}}_{\text{fast}}\hat{\mathbf{J}}(\mathbf{y}_{\text{slow}})\mathbf{y}_{\text{fast}} = -\hat{\mathbf{P}}_{\text{fast}}\mathbf{f}(\mathbf{y}_{\text{slow}})$$

$$\lambda \hat{P}_{\text{fast}} \hat{J}(\mathbf{y}_{\text{slow}}) \mathbf{y}_{\text{fast}} = -\hat{P}_{\text{fast}} \mathbf{f}(\mathbf{y}_{\text{slow}})$$

- We solve this equation for  $\mathbf{y}_{\text{fast}}$ .
- We can think of this system as a non-singular square system in the subspace related to  $\hat{P}_{\text{fast}}$ . It is a nondegenerate system because when considered in the  $\hat{P}_{\text{fast}}$  subspace, the system decays in all directions.
- Note that in  $1/\lambda$  order, the magnitude of  $\mathbf{y}_{\text{fast}}$  is determined by  $\hat{P}_{\text{fast}} \mathbf{f}$ . Hence,  $\mathbf{y}_{\text{fast}}$  is  $O(1/\lambda)$  distance from the manifold.

Average Distance from  $\mathbf{F}(\mathbf{y}) = 0$

After the system has decayed, the solution curve is at a distance of  $O(1/\lambda)$ .

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### Average Distance from $\mathbf{F}(\mathbf{y}) = \mathbf{0}$

After the system has decayed, the solution curve is at a distance of  $O(1/\lambda)$ .

- Consider the system  $\mathbf{y}' = \mathcal{F} = \lambda F + f$ , and project  $\mathbf{y}$  onto the closest point in the manifold.
- Let  $J_*$  be the Jacobian at the projected point  $\mathbf{y}_*$ .
- $\mathcal{J} = \lambda J + j = \lambda(J - J_*) + \lambda J_* + j$ .
  - By assumption,  $j$  represents the slow dynamics, so not much change is possible in a single time step.
  - Then  $\tau j = O(h)$ , since  $\tau = O(h)$ .
  - As before, the solution has essentially decayed to the manifold, so  $\mathbf{y} - \mathbf{y}_* = O\left(\frac{1}{\lambda}\right)$
  - Then  $J - J_* = O\left(\frac{1}{\lambda}\right)$ .

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- Then we have

$$\begin{aligned}
 e^{\tau \mathcal{J}} &= e^{\tau(\lambda J + j)} \\
 &= e^{\tau[\lambda(J - J_*) + \lambda J_* + j]} \\
 &= e^{\tau \lambda J_* + O(h)},
 \end{aligned}$$

where  $O(h)$  is from  $\lambda(J - J_*)$  and from  $j$ .

## Projectors

Then  $e^{\tau \mathcal{J}}$  is a projector into the slow dynamics up to exponentially small terms, which are neglected. Similarly for  $e^{\tau \tilde{\mathcal{J}}}$ .

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Then  $e^{\tau \mathcal{J}}$  is a projector into the slow dynamics up to exponentially small terms, which are neglected. Similarly for  $e^{\tau \tilde{\mathcal{J}}}$ .

- Consider the tolerance equation:

$$|\mathbf{y} - \bar{\mathbf{y}}| = \left| \int_0^{h/2} (e^{\tau \mathcal{J}} - e^{\tau \tilde{\mathcal{J}}}) d\tau e^{\frac{h}{2} \mathcal{J}} \mathcal{F} \right| \leq \text{TOL}$$

- One copy of  $h$  is obtained from the  $d\tau$  parameter; and another  $e^{\tau \mathcal{J}} - e^{\tau \tilde{\mathcal{J}}}$ .
- So then the local error is  $O(h^2)$ , which corresponds with a first order method.

### Order Reduction

In the stiff limit, the method suffers from an order reduction due to the rapid change allowed between the two projector matrices.

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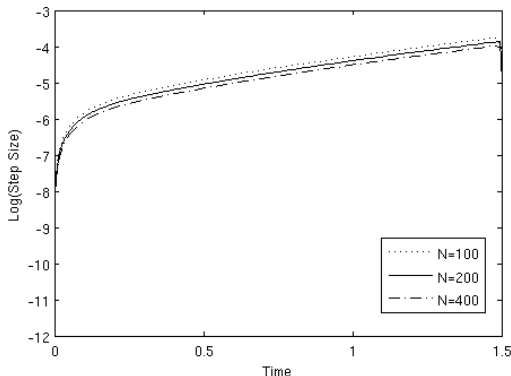
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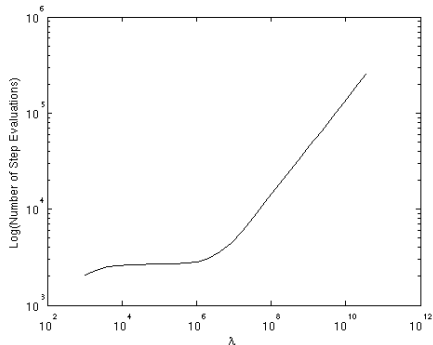
# Stiff Decay Characteristics

- Figure shows Log(Step Size) vs. Time for the equation  $u_t = u_{xx} - u^3$  with  $N=100$ ,  $N=200$ , and  $N=400$ ;  $t = 1.5$ .
- Step size does grow slightly with a larger number of points, however, the growth rate is linear for the period after decay of fast modes.



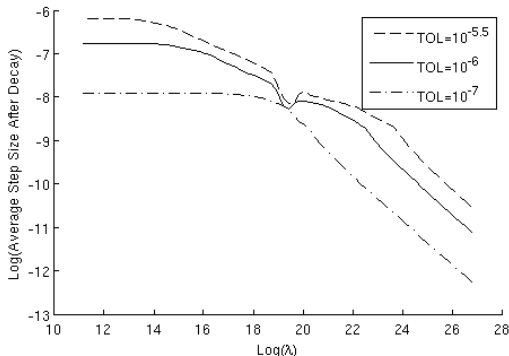
# Stiff Decay Characteristics

- Figure shows decay to a circle, with  $\text{Log}(\text{Number of Step Evaluations})$  vs.  $\lambda$ ,  $t = 3$ .
- Note that there is a period of non-changing step size for  $\lambda$  values between  $10^4$  and  $10^6$ .
- This period of constant step size indicates that the method exhibits stiff decay characteristics, but the increase after  $\lambda = 10^6$  is troubling.



## Dependence of Step Size on Tolerance Level

- Figure shows average step size after decay using different tolerance levels.
- Note that the plateau of non-increasing step size proceeds to the right for lower tolerance thresholds.

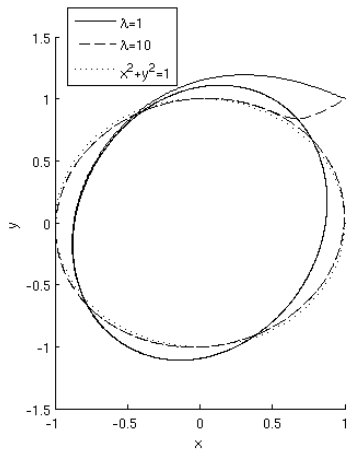


# Average Distance from $\mathbf{F}(\mathbf{y}) = \mathbf{0}$

- We expect the average distance from the stable manifold to be  $O(1/\lambda)$ .

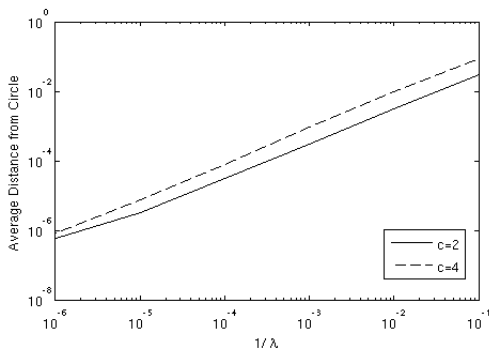
$$\begin{cases} \dot{x} = -y - \lambda x(x^2 + y^2 - 1) \\ \dot{y} = cx - \lambda y(x^2 + y^2 - 1) \end{cases}$$

- Now the dynamics push the solution curve toward an elliptical shape.
- Here,  $c = 2$ .



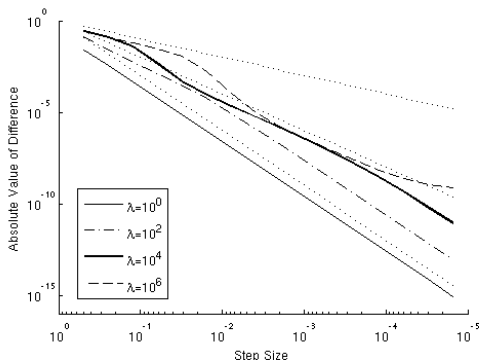
# Average Distance from $\mathbf{F}(\mathbf{y}) = \mathbf{0}$

**Figure:** Average distance from unit circle vs.  $1/\lambda$ , for multiple values of  $c$



# Reduction in Order

Figure:  $|\mathbf{y} - \bar{\mathbf{y}}|$ , obtained by one step of size  $h$ , and two steps of size  $h/2$ , respectively. Dotted lines indicate slopes of  $h, h^2, h^3$ .



## Concluding Remarks

- The method exhibits stiffness characteristics, but more numerical experimentation of the stiff limit is recommended.
- Ideally, this experimentation would be as independent of the choice of step size as possible.
- The code used for this research chooses step size based on the tolerance threshold; hence, step size is implicitly determined by the tolerance.
- Using estimation style analysis and numerical testing, we have shown that in the stiff limit, the method suffers an order reduction to first order.

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