# ***Software Development for Singular BVPs***


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# Problem class

Singular boundary value problems in ODEs

$$z'(t) = \frac{1}{t^\alpha} f(t, z(t)), \quad t \in (0,1], \quad \alpha \geq 1,$$

$$z'(\tau) = \tau^\beta f(\tau, z(\tau)), \quad \tau \in [1, \infty), \quad \beta \geq -1.$$

Problems on unbounded intervals: Transformation $t := 1/\tau$ yields

$$z'(t) = -\frac{1}{t^{\beta+2}} f(1/t, z(1/t)), \quad t \in (0,1].$$

Well-posedness related to boundary conditions ✓

# Bounded solutions

- Linear system, constant coefficient matrix

$$z'(t) = \frac{M}{t} z(t) + f(t), \;\; t \in (0,1], \;\; f \text{ smooth.}$$

- Linear system, variable coefficient matrix

$$z'(t) = \frac{M + tC(t)}{t} z(t) + f(t), \;\; t \in (0,1], \; f \text{ smooth.}$$

- Nonlinear problem

$$z'(t) = \frac{M + tC(t)}{t} z(t) + f(t, z(t)), \;\; t \in (0,1], \; f \text{ smooth.}$$

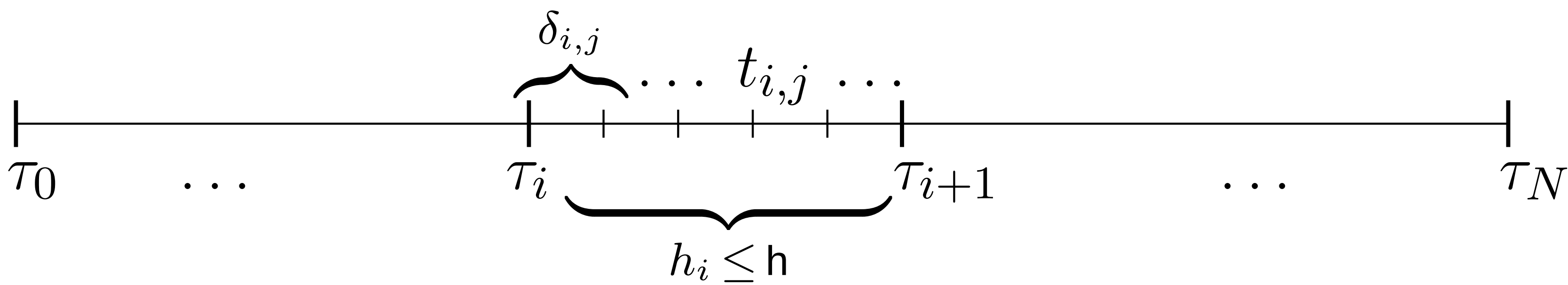
F. de Hoog and R. Weiss (1976)

# *Numerical approach*

- Collocation based on continuous, piecewise polynomial functions
- Error estimation
  - Defect correction $+$ backward Euler for singularity of the first kind ($\alpha = 1$)
  - Defect correction $+$ box scheme for essential singularity ($\alpha > 1$, unbounded intervals)
  - Mesh halving for general purpose (higher order, implicit, DAEs)
- Adaptive mesh selection based on equidistribution of the global error

# *Collocation methods*

$$z'(t) - F(t, z(t)) = 0 \text{ plus BC}$$




- Globally continuous, piecewise polynomial function $p(t)$ of maximal degree $m$ satisfying

$$p'(t_{i,j}) - F(t_{i,j}, p(t_{i,j})) = 0 \text{ plus BC}.$$

Convergence regular case:

- stage order: $\|p - z\|_\infty = O(\mathsf{h}^m)$,
- superconvergence at $\tau_i$.

# *Error estimate*

$$p'(t_{i,j}) - F(t_{i,j}, p(t_{i,j})) = 0 \text{ plus BC}$$

- Classical idea due to Zadunaisky, Frank, Stetter (1975-1978)

  Modification: Auzinger, Koch, Weinmüller (2001-2002).

- Auxiliary scheme for OP: BEUL

$$\frac{\xi_{i,j} - \xi_{i,j-1}}{\delta_{i,j}} = F(t_{i,j}, \xi_{i,j}) \quad + \quad \text{BC}.$$

- Neighboring scheme: BEUL

$$\frac{\pi_{i,j} - \pi_{i,j-1}}{\delta_{i,j}} = F(t_{i,j}, \pi_{i,j}) + \bar{d}_{i,j} \quad + \quad \text{BC}.$$

- Error estimate: $p(t_{i,j}) - z(t_{i,j}) \approx \pi_{i,j} - \xi_{i,j}, \quad \forall i, j$

# Theoretical results

- Convergence of collocation of degree $m$
  - Singularity of first kind: $O(\mathsf{h}^m)$ $\checkmark$
  - Essential singularity: $O(\mathsf{h}^m)$
- Asymptotical correctness of error estimates
  - Singularity of first kind: $O(\mathsf{h}^{m+1})$ $\checkmark$
  - Essential singularity:
    $O(\mathsf{h}^{m+\gamma}), \quad 0 < \gamma = \gamma(\alpha) < 1$
- Asymptotical equidistribution of the global error
  $\max_{t \in J_i}(p(t) - z(t)) = \text{const}(1 + O(\mathsf{h}))$ $\checkmark$

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# *Collocation software*

- sbvp – MATLAB code for explicit first order problems, available from `http://www.math.tuwien.ac.at/~ewa/`
  - Error estimation and mesh selection
  - Variable collocation degree $m = 1 \ldots 8$
  - Runge-Kutta basis for polynomial representation – reduction of roundoff error
  - Efficient, Newton-based solver for nonlinear collocation equations
  - Rescaling of linear equations for favorable conditioning
  - Vectorization for efficient computations

# *Collocation software(2)*

- Further development – sbvp
  - Eigenvalue problems
  - “Pathfollowing” (turning points)
  - Implicit formulation, DAEs
- New development – MATLAB collocation solver
  - Mixed order ODEs (order zero to four)
  - Unknown parameters
  - Implicit formulation, DAEs

# Applications – NLS

Cubic nonlinear Schrödinger equation

$$\mathrm{i}\frac{\partial u}{\partial t} + \Delta u + |u|^2 u = 0,\ t > 0, \quad u(x,0) = u_0(x),\ x \in \mathbb{R}^d.$$

Applications: Plasma physics, nonlinear optics
Self-similar blow-up solutions can be computed from

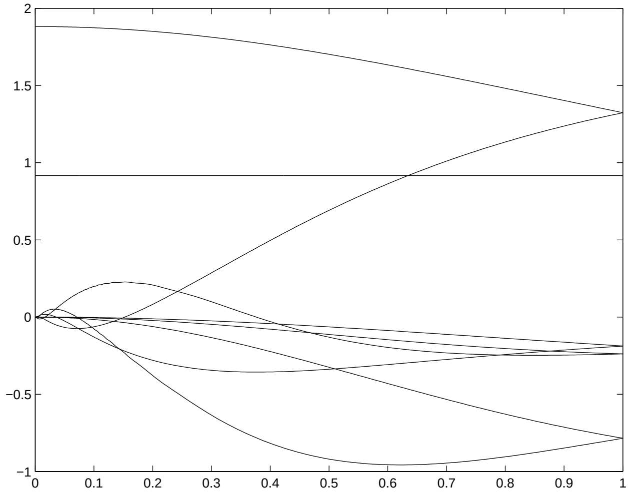
$$z''(\tau) + \frac{2}{\tau} z'(\tau) - z(\tau) + \mathrm{i}a(\tau z(\tau))' + |z(\tau)|^2 z(\tau) = 0,\ \ \tau > 0.$$

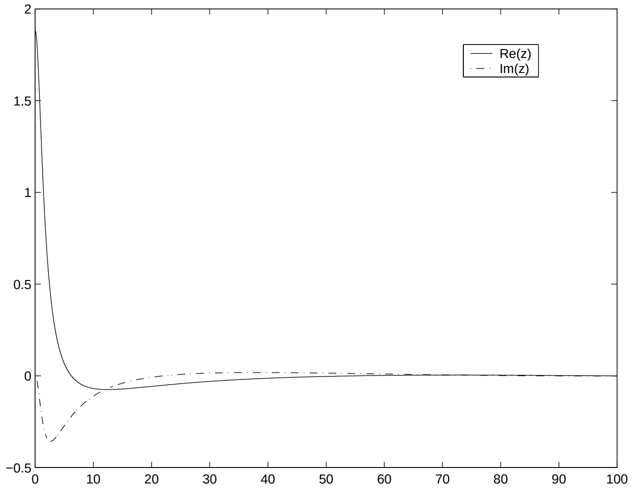
- Transformation to nine first order ODEs on $(0,1]$
- Slowly varying solutions $\Rightarrow$ Singularity of first kind

# Applications – NLS(2)

Numerical solution from our MATLAB code sbvp:

- $AbsTol = RelTol = 5 \cdot 10^{-5}$
- 256 subintervals on $[0, 1]$
- step-size ratio 9.71





# Applications – Parab. Eqns.

Quasilinear parabolic problem

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(u^\sigma \frac{\partial u}{\partial x}\right) + u^\beta, \qquad t > 0.$$

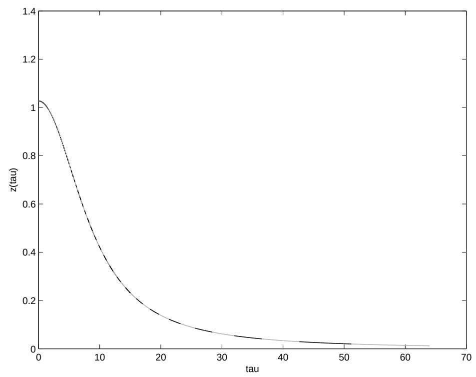
Application: Model for a temperature profile of a fusion reactor plasma with one source term.
Self-similar blow-up solutions:

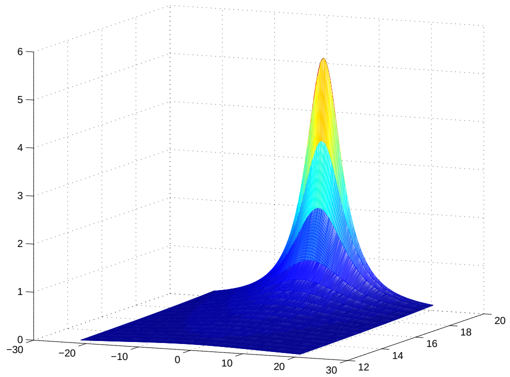
$$(z^\sigma(\tau)z'(\tau))' - m\tau z'(\tau) - \frac{1}{\beta - 1} z(\tau) + z^\beta(\tau) = 0, \quad \tau > 0.$$

This ODE can be solved directly by our new code!

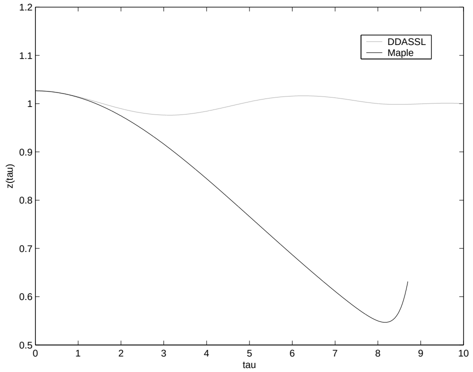
# *Applications – Parab. Eqns.*

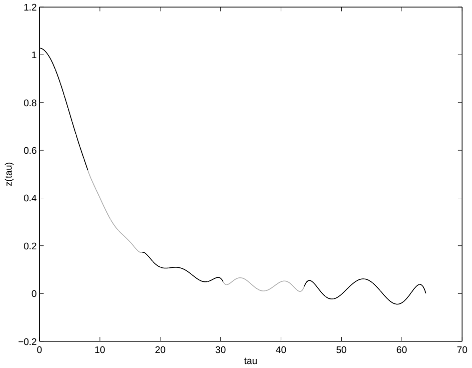
Correct solution profile by our approach:



Shooting approach and truncated interval:



# *Conclusions*

We can currently solve

1. Singularity of the first kind ($\alpha = 1$)
2. Essential singularity ($\alpha > 1$)
3. Unbounded intervals

- With error estimation and mesh selection
  - Explicit first order problems
- By collocation on fixed grid
  - Mixed order up to four
  - Implicit problems
  - DAEs
  - Unknown parameters

# *Outlook*

- Equip the new solver with error estimation (mesh halving) and mesh selection
- Pathfollowing for parameter-dependent problems, pseudo-arclength parametrization!
- Complex Ginzburg-Landau equation – perturbation of NLS, turning points!
- Further applications

# *Software Development for Singular BVPs*

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# Conv. proof - difficulties

Case study: Consider linear system

$$z'(t) - \frac{D}{t} z(t) = f(t), \quad t \in (0,1], \quad D = \text{diag}(-1,2)$$

$$z_1(0) = 0, \quad z_2(1) = \beta.$$

Box scheme on equidistant mesh, $h = 1/N$:

$$\frac{\xi_i - \xi_{i-1}}{h} - \frac{D}{t_{i-1/2}} \frac{\xi_i + \xi_{i-1}}{2} = f_{i-1/2}, \, i = 1, \ldots, N$$

$$\xi_{1,0} = 0, \, \xi_{2,N} = \beta.$$

Question! Convergence $\lim_{h \to 0} \|\xi_h - z_{\Delta_h}\| = 0$?
$\xi_h := (\xi_0, \ldots, \xi_i, \ldots, \xi_N)$
$z_{\Delta_h} := (z(0), \ldots, z(t_i), \ldots, z(1)).$

# Conv. proof - difficulties(2)

Classical approach:
Stability + Consistency = Convergence!

- Write the scheme as

$$\Phi_h[\xi_h] = f_h, \;\; \Phi_h : \mathbb{R}^{2(N+1)} \longrightarrow \mathbb{R}^{2(N+1)}.$$

- Show that $\Phi_h^{-1}$ exists.
- Show stability: $\|\xi_h - \eta_h\| \leq S\,\|\Phi_h[\xi_h] - \Phi_h[\eta_h]\|$ for $h$ sufficiently small and $S \neq S(h)$.

  Means that $\Phi_h$ is one to one mapping.
- Consistency: For $z$ sufficiently smooth

$$\frac{z(t_i) - z(t_{i-1})}{h} - D\frac{z(t_i) + z(t_{i-1})}{2} = f_{i-1/2} + O(h^2).$$

# Conv. proof - difficulties(3)

- Consequently, $\Phi_h[\xi_h] = f_h, \;\; \Phi_h[z_{\Delta_h}] = f_h + O(h^2) \;\Rightarrow$
- Stability + Consistency = Convergence!

$$\|\xi_h - z_{\Delta_h}\| \le S\,\|\Phi_h[\xi_h] - \Phi_h[z_{\Delta_h}]\| \le S\,h^2.$$

- Difficulty in singular case:

$$\frac{z(t_i) - z(t_{i-1})}{h} - \frac{D}{t_{i-1/2}}\,\frac{z(t_i) + z(t_{i-1})}{2} = f_{i-1/2} + O\left(\frac{h^2}{t_{i-1/2}}\right).$$

- Remedy: (1) Invert $\Phi_h: \;\; \Phi_h[\xi_h] = f_h \;\Rightarrow\; \xi_h = \Phi_h^{-1} f_h$

(2) $\xi_h - z_{\Delta_h} = \Phi_h^{-1}(\Phi_h[\xi_h] - \Phi_h[z_{\Delta_h}]) = \Phi_h^{-1} O\left(\frac{h^2}{t_{i-1/2}}\right) = O(h^2).$

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# Bounded solutions

Case study $\alpha = 1$: Consider linear scalar problem

$$z'(t) = \underbrace{\frac{\lambda}{t} z(t) + f(t),}_{F(t,z(t))} \quad t \in (0,1], \quad \lambda \in \mathbb{R},\ f \in C[0,1].$$

We are interested in bounded solutions

$$z \in C[0,1]: \qquad z(t) = z_h(t) + z_p(t).$$

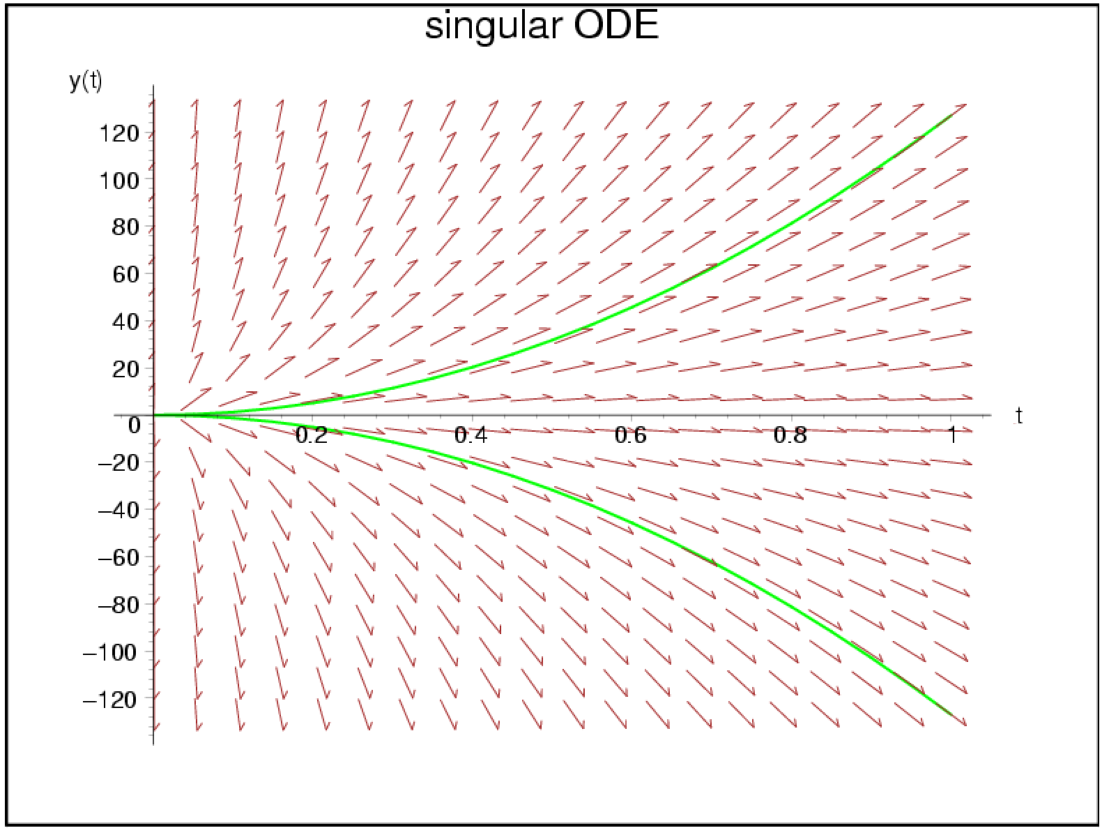
Difficulties:

- $F(t, z(t))$ is not Lipschitz continuous uniformly in $t$.
- It depends on $\lambda$ whether bounded nontrivial solution exists.

# Bounded solutions(2)

General solution of the homogeneous problem:

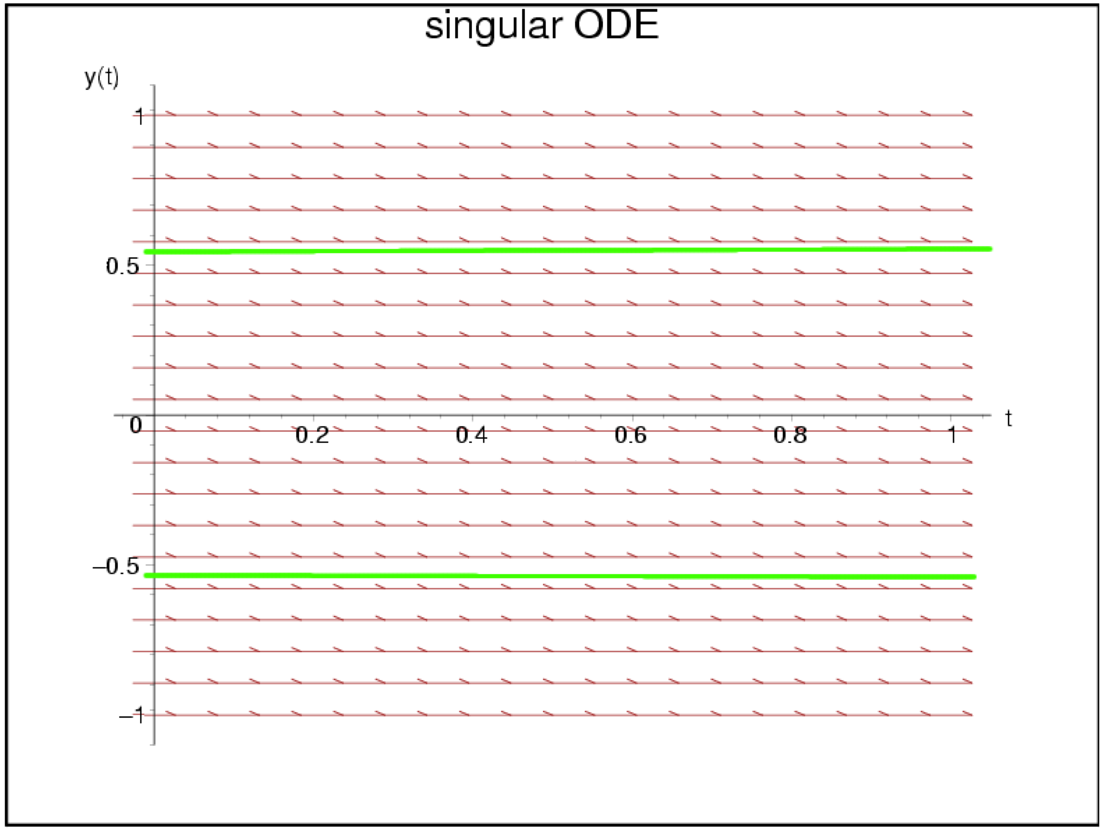
$$z_h(t) = c\,t^{\lambda}, \quad \lambda > 0$$



# *Bounded solutions(3)*

General solution of the homogeneous problem:

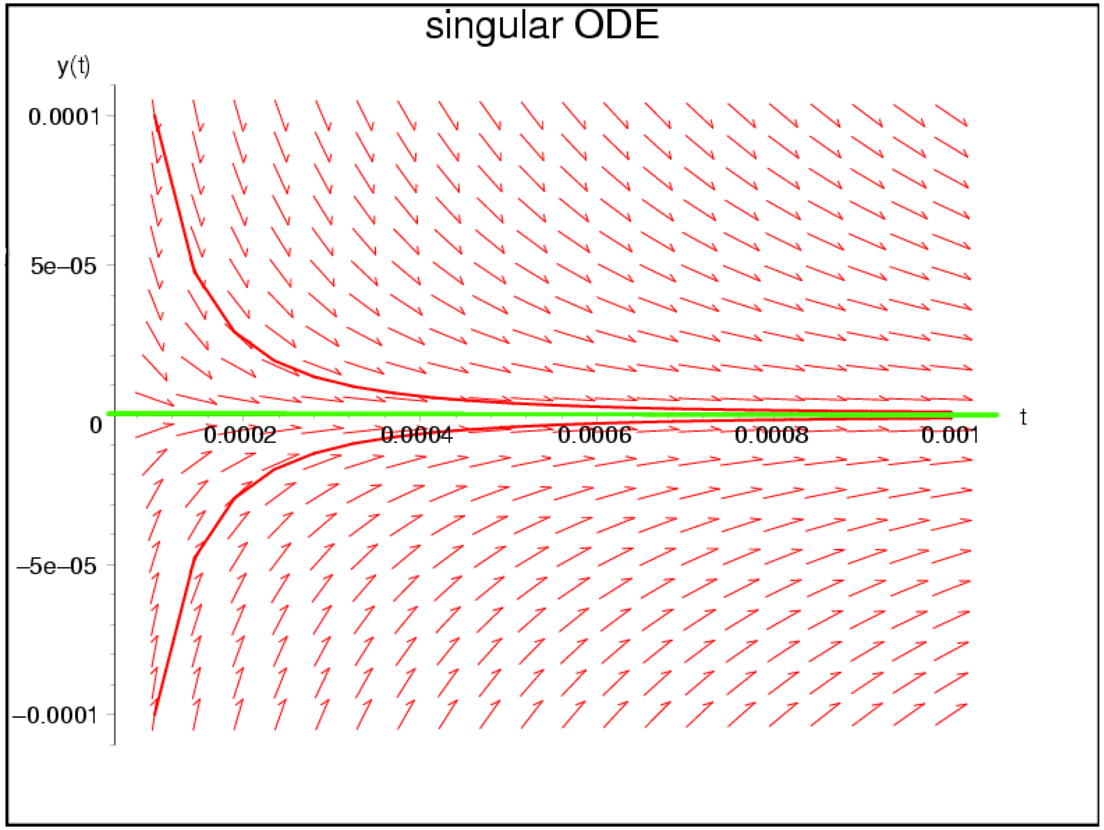
$$z_h(t) = c\,t^\lambda \;\Rightarrow\; z_h(t) = c, \quad \lambda = 0$$



# *Bounded solutions(4)*

General solution of the homogeneous problem:

$$z_h(t) = c\,t^{\lambda} \;\Rightarrow\; z_h(t) = 0, \quad \lambda < 0$$



## *Bounded solutions(5)*

Particular solution of the inhomogeneous problem:

$$z'(t) = \frac{\lambda}{t} z(t) + f(t), \quad t \in (0,1], \quad \lambda \in \mathbb{R}, \; f \in C[0,1].$$

$\lambda$ and $f \in C[0,1] \quad \Rightarrow z_p \in C[0,1]$ and $z_p(0) = 0.$

- $\lambda \geq 0 \qquad z(t) = c\,t^{\lambda} + z_p(t) \in C[0,1]$
  Prescribe $z(1) := \zeta$ to fix $c$.
  In general $z \in C^1(0,1]$.
- $\lambda < 0 \qquad z(t) = z_p(t) \in C[0,1]$
  Require $z(0) := 0$ for $z \in C[0,1]$.
  In general $z \in C^1[0,1]$.