## Boundary value problems with very sharp structures: numerical challenges



Theodore Kolokolnikov, Dalhousie University


## Introduction

- Singular perturbation problems depend on a small parameter $\varepsilon$ which typically premultiplies the highest derivative.
- As $\varepsilon \rightarrow 0$, the problems exhibit localized structures such as boundary layers, corner layers, spikes, interfaces.
- Typically, the localized structure has the size $O(\varepsilon)$; the solution is relatively smooth outside the localized region.
- Standard codes to solve BVP may have difficulty resolving localized structures: typically, meshsize scales with $1 / \varepsilon$.
- Example: a standard code requires 10,000 meshpoints when $\varepsilon=10^{-5}$ ?


## Problem 1

Solve the problem

$$
\varepsilon^{2} u^{\prime \prime}-u+\left(1+x^{2}\right) u^{2}=0 ; \quad u^{\prime}(0)=0 ; \quad \varepsilon u^{\prime}(1)=-u(1) .
$$

Asymptotic solution: Transform

$$
\begin{gathered}
x=\varepsilon y \\
u_{y y}-u+\left(1+\varepsilon^{2} y^{2}\right) u^{2}
\end{gathered}
$$

so that

$$
u(x) \sim w\left(\frac{x}{\varepsilon}\right)
$$

where
$w=\frac{3}{2} \operatorname{sech}^{2}(y / 2)$ solves $w_{y y}-w+w^{2}=0.0$.


- Note that

$$
w \sim O(1) \text { for } y=O(1)
$$

but it decays,

$$
w \sim 6 e^{-y} \text { for large } y
$$

- This exponential decay can cause trouble for BVP solvers.
- The solution exhibits two different spatial scales.
- Maple BVP solver: meshsize scales like $1 / \varepsilon$.
- Matlab does much better [see below]


## Split-range method

Split-range method

- Choose $l \in[0,1]$,

$$
\varepsilon \ll l \ll 1
$$

- On $[0, l]$, (inner problem) transform:

$$
x=l y, u(t)=\hat{u}(y)
$$

- On $[l, 1]$, (outer problem) transform:

$$
x=l+(1-l) y, u(t)=\exp \left(\frac{\tilde{u}(y)}{\varepsilon}\right)
$$

- We get a 4-dimensional $B V P$ for $\hat{u}, \tilde{u}$ on $y \in[0,1]$. The boundary conditions become:

$$
\begin{aligned}
\hat{u}^{\prime}(0) & =0, \quad \tilde{u}^{\prime}(1)=-1 \\
\hat{u}(1) & \left.=\exp \left(\frac{\tilde{u}(0)}{\varepsilon}\right) \quad \text { (continuity of } u\right) \\
\frac{\hat{u}^{\prime}(1)}{l} & \left.=\frac{1}{\varepsilon(1-l)} \exp \left(\frac{\tilde{u}(0)}{\varepsilon}\right) \tilde{u}^{\prime}(0) \text { (continuity of } u^{\prime}\right)
\end{aligned}
$$

- The parameter $l$ is chosen by trial and error. Global tolerance is set to $10^{-6}$; Maple's dsolve/bvp is used with adaptive gridding.


## Meshsize scaling laws

| $\varepsilon$ | split range <br> $(l=9 \varepsilon)$ | split range <br> $\left(l=4 \varepsilon \ln \frac{1}{\varepsilon}\right)$ | Standard Maple <br> (adaptive mesh) | Standard Matlab <br> (adaptive mesh) |
| :--- | :--- | :--- | :--- | :--- |
| 0.1 | 21 | 21 | 51 | 50 |
| 0.05 | 21 | 24 | 87 | 37 |
| 0.025 | 21 | 21 | 106 | 41 |
| $2^{-3} \times 0.1$ | 21 | 26 | 178 | 38 |
| $2^{-4} \times 0.1$ | 21 | 29 | 376 | 41 |
| $2^{-5} \times 0.1$ | 30 | 30 | 792 | 42 |
| $2^{-6} \times 0.1$ | 58 | 32 | error | 50 |
| $2^{-7} \times 0.1$ | 119 | 31 |  | 39 |
| $2^{-8} \times 0.1$ | 226 | 32 |  | 35 |
| $2^{-9} \times 0.1$ | 472 | 33 |  | 35 |
| $2^{-10} \times 0.1$ | 946 | 34 |  | 93 |
| $2^{-11} \times 0.1$ | error | 35 |  | 61 |
| $\ldots$ |  | $\ldots$ |  | $\ldots$ |
| $2^{-16} \times 0.1$ |  | 41 |  | 36 |
| $2^{-17} \times 0.1$ |  | 42 |  | 38 |

- The "good" $l$ scales like $l=O(\varepsilon \ln \varepsilon)$ !


## Understanding $l=O(\varepsilon \ln \varepsilon)$

- Consider a simple problem

$$
\begin{equation*}
\varepsilon u_{x x}+u_{x}=1, \quad u(0)=0=u(1) \tag{1}
\end{equation*}
$$

- Asymptotic composite solution is:

$$
\begin{equation*}
u \sim \exp (-x / \varepsilon)+x-1 \tag{2}
\end{equation*}
$$

- There is a boundary layer at 0 as $\varepsilon \rightarrow 0$ :



## Error analysis, uniform mesh

- Discretize: let $h=1 / N$ and approximate $\varepsilon u_{x x}+u_{x}=1$ by

$$
\varepsilon \frac{\hat{u}_{i-1}+\hat{u}_{i+1}-2 u_{i}}{h^{2}}+\frac{\hat{u}_{i+1}-\hat{u}_{i-1}}{2 h}=1 ; \quad \hat{u}_{0}=0=\hat{u}_{N} .
$$

- Interpolate $\hat{u}$ so it is defined on the whole interval $[0,1]$ with $\hat{u}(i h)=\hat{u}_{i}$.
- Next, note that

$$
\begin{aligned}
\frac{\hat{u}_{i+1}+\hat{u}_{i-1}-2 \hat{u}_{i}}{h^{2}} & =\hat{u}^{\prime \prime}+h^{2} \frac{\hat{u}^{\prime \prime \prime \prime}}{12}+O\left(h^{4}\right) ; \\
\frac{\hat{u}_{i+1}-\hat{u}_{i-1}}{2 h} & =\hat{u}^{\prime}+h^{2} \frac{\hat{u}^{\prime \prime \prime}}{6}+O\left(h^{4}\right)
\end{aligned}
$$

- So consider the error

$$
w=u-\hat{u}
$$

Then

$$
\begin{aligned}
\varepsilon w_{x x}+w_{x} & \sim h^{2}\left(\varepsilon \frac{\hat{u}^{\prime \prime \prime \prime}}{12}+\frac{\hat{u}^{\prime \prime \prime}}{6}\right) \\
& \sim h^{2}\left(\varepsilon \frac{u^{\prime \prime \prime \prime}}{12}+\frac{u^{\prime \prime \prime}}{6}\right) \\
& \sim-\frac{1}{12} \frac{h^{2}}{\varepsilon^{3}} \exp (-x / \varepsilon)
\end{aligned}
$$

- The error $w=u-\hat{u}$ satisfies

$$
\varepsilon w_{x x}+w_{x} \sim-\frac{1}{12} \frac{h^{2}}{\varepsilon^{3}} \exp (-x / \varepsilon) ; \quad w(0)=0=w(1)
$$

Note the resonance! The solution is

$$
w \sim \frac{1}{12} \frac{h^{2}}{\varepsilon^{3}} x \exp (-x / \varepsilon)
$$

Maximum occurs at $x=\varepsilon$; max error is

$$
\max w=\left(\frac{h}{\varepsilon}\right)^{2} \frac{e^{-1}}{12}
$$

Conclusion: $N=O(1 / \varepsilon)$ for uniform mesh!!!

## A two-sized mesh:

Take $l \in(0,1)$ and discretize using uniform mesh of $N_{1}$ points inside $[0, l]$ and another uniform mesh of $N_{2}=N-N_{1}$ points inside $[l, 1]$.

The error function $w=u-\hat{u}$ then satisfies:

$$
\varepsilon w^{\prime \prime}+w^{\prime} \sim-\frac{1}{12}\left\{\begin{array}{cl}
\frac{l^{2}}{N_{1}^{2} \varepsilon^{3}} e^{-x / \varepsilon}, & x \in(0, l) \\
\frac{(1-l)^{2}}{N_{2}^{2} \varepsilon^{3}} e^{-x / \varepsilon}, & x \in(l, 1)
\end{array}\right.
$$

Define

$$
r:=N_{2} / N_{1} ;
$$

and write

$$
N_{1}=N \frac{1}{1+r} ; \quad N_{2}=N \frac{r}{1+r}
$$

Assuming $l, \varepsilon \ll 1$, solving for $w$ we obtain:

$$
\begin{aligned}
w & \sim \frac{1}{12} \frac{(1+r)^{2}}{N^{2}}\left\{e^{-x / \varepsilon} \frac{x l^{2}}{\varepsilon^{3}}+e^{-l / \varepsilon} \frac{l^{2}}{\varepsilon^{2}}\left(\frac{1}{r^{2}} \frac{1}{l^{2}}-1\right)\left(1-e^{-x / \varepsilon}\right)\right\}, x \in[0, l] \\
& \sim \frac{1}{12} \frac{(1+r)^{2}}{N^{2}}\left\{\frac{e^{-x / \varepsilon}}{r^{2}} \frac{x}{\varepsilon^{3}}+\left(1-\frac{1}{r^{2} l^{2}}\right) \frac{l^{2} e^{-x / \varepsilon}}{\varepsilon^{2}}\left(e^{-l / \varepsilon}-1+\frac{l}{\varepsilon}\right)\right\}, x \in[l, 1]
\end{aligned}
$$

Given $\varepsilon, N$, we want to determine $l, r$ which minimizes the maximum of $w$.

The proper scaling is

$$
l=\varepsilon \ln \frac{1}{\varepsilon} p
$$

The maximum of $w$ is attained at $x^{\star} \sim \varepsilon \ll l$; given by

$$
w\left(x^{\star}\right) \sim \frac{1}{12} \frac{(1+r)^{2}}{N^{2}}\left\{\exp (-1)\left(\ln \frac{1}{\varepsilon}\right)^{2} p^{2}+\varepsilon^{p-2} \frac{1}{r^{2}}(1-\exp (-1))\right\}
$$

Minimizing with respect to $p$ and $r$, we get:

$$
\begin{gathered}
p=2 ; r=\left(\frac{e-1}{4}\right)^{1 / 3}\left(\frac{1}{\ln (1 / \varepsilon)}\right)^{2 / 3} ; \\
\min _{l, r} \max _{x} w \sim \frac{1}{3 e}\left(\frac{\ln \frac{1}{\varepsilon}}{N}\right)^{2}
\end{gathered}
$$

Conclusion: $N=O(\ln (1 / \varepsilon))$ for two-sized mesh!!! [this is exponentially better than $N=O(1 / \varepsilon)$ scaling of the uniform mesh!!ç

Example 1: $\varepsilon:=10^{-8} ; N=200$.

- The optimal two-sized mesh is:

$$
\begin{aligned}
l & =3.6 \times 10^{-6} \\
r & =0.108 \Longrightarrow N_{1}=180, N_{2}=20
\end{aligned}
$$

- Numerical error $=0.0013$. Predicted error $=0.0014$. Uniform mesh: Would need $N=10^{9}$ meshpoints to get same accuracy!

Example 2: Direct comparison of uniform vs. split-range:

| $\varepsilon$ | $N$ | error <br> (unif. mesh) | error <br> (optimal two-sided mesh) |
| :--- | :--- | :--- | :--- |
| 0.02 | 100 | 0.0080 | 0.00053 |
| 0.01 | 100 | 0.035 | 0.00072 |
| 0.005 | 100 | 0.14 | 0.00092 |
| 0.0025 | 100 | FAIL | 0.0011 |
| $10^{-3}$ | 100 |  | 0.0012 |
| $10^{-4}$ | 100 |  | 0.0028 |
|  |  |  |  |
| $10^{-6}$ | 100 |  | 0.0031 |
| $10^{-6}$ | 200 |  | 0.00082 |

## Problem 2

Same ODE as problem 1:

$$
\varepsilon^{2} u^{\prime \prime}-u+\left(1+x^{2}\right) u^{2}=0 ; \quad u^{\prime}(0)=0 ; \quad \varepsilon u^{\prime}(1)=-u(1) .
$$

but it has another solution of the form $u=w\left(\frac{x-x_{0}}{\varepsilon}\right)$ where $x_{0}$ is approximately scales like

$$
x_{0} \sim \varepsilon \frac{1}{2} \ln \left(\frac{30}{\varepsilon x_{0}}\right)+O(1 / \ln (\varepsilon))
$$



## Three different scales

- To leading order, $x_{0} \sim \frac{1}{2} \varepsilon \ln (30 / \varepsilon)$ has $O(\varepsilon \ln 1 / \varepsilon)$
- The extent of the spike has $O(\varepsilon)$
- The outer problem has extend $O(1)$
- The relative error in the asymptotics of $x_{0}$ is $O\left(1 / \ln \varepsilon^{-1}\right)$;
- This means that to asymptotics with numerics, we must take $1 / \ln \varepsilon^{-1} \sim 0.1 \Longrightarrow$ $\varepsilon \sim 10^{-5!!!!}$
- Challenge: can you compute with $\varepsilon \sim 10^{-4}$ ?
- Maple, matlab all fail for this problem when $\varepsilon \sim 10^{-3}$.


## Problem 3

$$
\begin{equation*}
0=u_{r r}+\frac{2}{r} u_{r}-u+u^{2}(\varepsilon+r), \quad u^{\prime}(0)=0, u^{\prime}(\infty)=0 \tag{3}
\end{equation*}
$$

- THEOREM: In the limit $\varepsilon \ll 1$, Let $r_{0} \gg 1$ be the large solution to the equation

$$
\varepsilon \sim 30 r_{0}^{2} \exp \left(-2 r_{0}\right)
$$

Then there exists solutions of (3) of the form

$$
u(r) \sim \frac{1}{r_{0}} w\left(r-r_{0}\right)
$$

- Error is expected to be of $O(1 / \ln (1 / \varepsilon))$. To validate results, must take extemely small $\varepsilon$; for example if $\varepsilon=10^{-3}$ then $r_{0} \sim 5$, is not so small
- Standard codes [matlab, maple] all fail even for $\varepsilon=10^{-2}\left[r_{0} \sim 5.5\right]$.


## Solve for $\varepsilon$ instead

- Instead of fixing $\varepsilon$ and solving for $r_{0}$, fix $r_{0}$ then solve numerically the problem (3) first on $\left[0, r_{0}\right]$ with $u^{\prime}\left(r_{0}^{+}\right)=0$ and on $\left[r_{0}, \infty\right]$; with $u^{\prime}\left(r_{0}^{-}\right)=0$.
- Additional constraint $u\left(r_{0}^{-}\right)=u\left(r_{0}^{+}\right)$determines $\varepsilon$.
- Can get an accurate answer up to $r_{0} \sim 9.5$. The method fails for bigger values of $r_{0}$ since the difference between $u\left(r_{0}^{-}\right)-u\left(r_{0}^{+}\right)$becomes smaller than the machine tolerance.

| $r_{0}$ | $\varepsilon$ | Solution $r_{0}$ to <br> $\varepsilon=30 r_{0}^{2} e^{-2 r_{0}}$ | \%err |
| :--- | :--- | :--- | :--- |
| 4 | 0.05544 | 4.603 | $15.09 \%$ |
| 4.5 | 0.02965 | 5.018 | $11.52 \%$ |
| 5 | 0.015065 | 5.451 | $9.02 \%$ |
| 5.5 | 0.007326 | 5.898 | $7.24 \%$ |
| 6 | 0.003441 | 6.357 | $5.95 \%$ |
| 6.5 | 0.001569 | 6.825 | $5.00 \%$ |
| 7 | 0.0007028 | 7.297 | $4.25 \%$ |
| 7.5 | 0.0003080 | 7.776 | $3.68 \%$ |
| 8 | 0.0001336 | 8.256 | $3.20 \%$ |
| 8.5 | $5.704 \mathrm{e}-5$ | 8.74 | $2.83 \%$ |
| 9 | $2.41 \mathrm{e}-5$ | 9.227 | $2.52 \%$ |

## Discussion

- When splitting the integration range, take the splitting point to have order $l=O(\varepsilon \ln \varepsilon)$
- Problems with sharp interior boundary layers whose location depends on $\varepsilon$ are difficult for standard solvers
- Matlab bvp solver is currently better than maple's [as of Aug 2010]
- The asymptotics of the problem should be reflected in the numerics; the analytical insight is invaluable when looking for numerical solution, especially for nonlinear problems.

