



Diagramme erstellen mit pgfplots

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Motivation / Ziel

■ Motivation

- ... alles aus einem Guss
- aber warum dann GNUplot-Diagramme einbinden?

■ Ziel

- Diagramme für einen Artikel
- schwarz/weiß-Diagramme
- nicht jeden Befehl merken



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Grundlagen

- Paket laden

```
1 \input pgfplots.tex % Plain TeX
  \usepackage{pgfplots} % LaTeX
  \usemodule[pgfplots] % ConTeXt
```

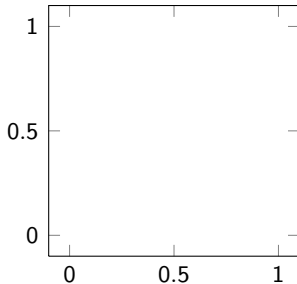
Grundlagen

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```
1 \input pgfplots.tex % Plain TeX
  \usepackage{pgfplots} % LaTeX
  \usemodule[pgfplots] % ConTeXt
```

■ Standardachse

```
1 \begin{tikzpicture}
  \begin{axis}
    % Plot code
  \end{axis}
5 \end{tikzpicture}
```



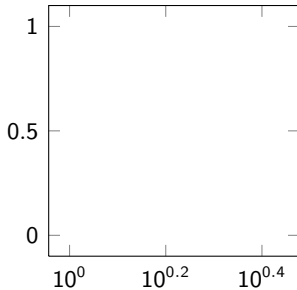
Grundlagen

■ Paket laden

```
1 \input pgfplots.tex % Plain TeX
  \usepackage{pgfplots} % LaTeX
  \usemodule[pgfplots] % ConTeXt
```

■ logarithmische x-Achse

```
1 \begin{tikzpicture}
  \begin{semilogxaxis}
    % Plot code
  \end{semilogxaxis}
5 \end{tikzpicture}
```



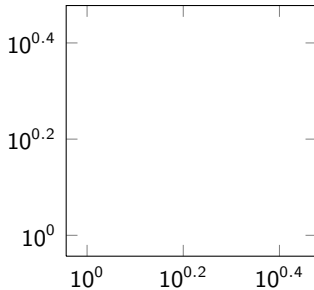
Grundlagen

■ Paket laden

```
1 \input pgfplots.tex % Plain TeX
  \usepackage{pgfplots} % LaTeX
  \usemodule[pgfplots] % ConTeXt
```

■ logarithmische Achsen

```
1 \begin{tikzpicture}
  \begin{loglogaxis}
    % Plot code
  \end{loglogaxis}
5 \end{tikzpicture}
```



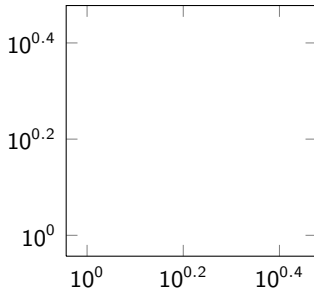
Grundlagen

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```
1 \input pgfplots.tex % Plain TeX
  \usepackage{pgfplots} % LaTeX
  \usemodule[pgfplots] % ConTeXt
```

■ logarithmische Achsen

```
1 \begin{tikzpicture}
  \begin{loglogaxis}
    % Plot code
  \end{loglogaxis}
5 \end{tikzpicture}
```



■ „neue“ Verbesserungen nutzen

```
1 \pgfplotsset{compat = newest}
```

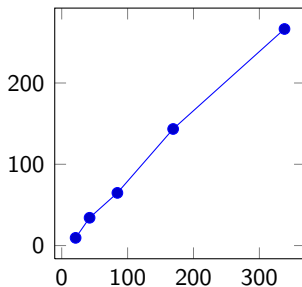


Kleiner Datensatz

Concentration / mmol dm^{-3}	Rate / s^{-1}
338.1	266.45
169.1	143.43
84.5	64.80
42.3	34.19
21.1	9.47

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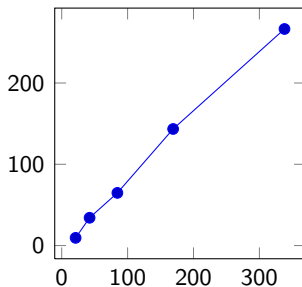


```

1 \addplot coordinates {
    ( 338.1, 266.45 )
    ( 169.1, 143.43 )
    ( 84.5, 64.80 )
5 ( 42.3, 34.19 )
    ( 21.1, 9.47 )
};
  
```

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Concentration / mmol dm^{-3}	Rate / s^{-1}
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```

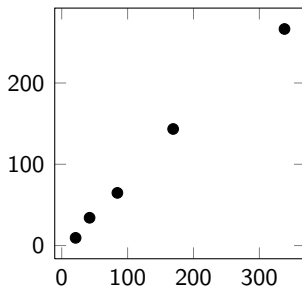
1 \addplot coordinates {
    ( 338.1, 266.45 )
    ( 169.1, 143.43 )
    ( 84.5, 64.80 )
5 ( 42.3, 34.19 )
    ( 21.1, 9.47 )
};

```

- keine Farbe
- keine Linien

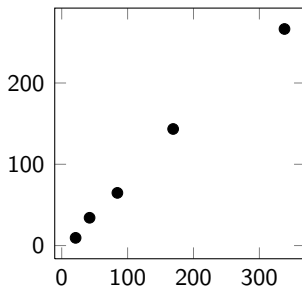
Kleiner Datensatz

```
1 \addplot[
    color = black,
    fill = black,
    mark = *,
5    only marks
] coordinates {
    ( 338.1, 266.45 )
    ( 169.1, 143.43 )
    ( 84.5, 64.80 )
10  ( 42.3, 34.19 )
    ( 21.1, 9.47 )
};
```



Kleiner Datensatz

```
1 \addplot[
    color = black,
    fill = black,
    mark = *,
5    only marks
] coordinates {
    ( 338.1, 266.45 )
    ( 169.1, 143.43 )
    ( 84.5, 64.80 )
10  ( 42.3, 34.19 )
    ( 21.1, 9.47 )
};
```



- Trendlinie hinzufügen

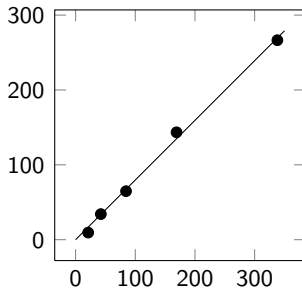
Kleiner Datensatz

```

1  \addplot[
    color = black,
    fill  = black,
    mark  = *,
5     only marks
] coordinates { ... };

\addplot[
10  color = black,
    mark  = none
]
    coordinates {
        ( 0, 0 )
        ( 350, 279 )
15  };

```



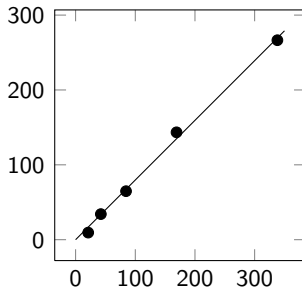
Kleiner Datensatz

```

1  \addplot[
    color = black,
    fill  = black,
    mark  = *,
5     only marks
] coordinates { ... };

\addplot[
10  color = black,
    mark  = none
]
    coordinates {
        ( 0, 0 )
        ( 350, 279 )
15  };

```

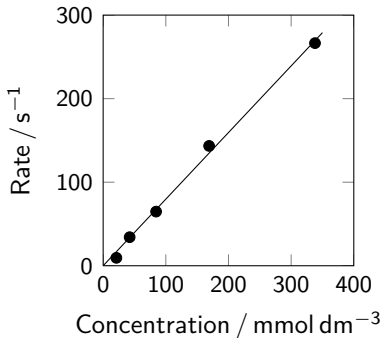


- Achsen beschriften
- Achsenlimits anpassen

Kleiner Datensatz

```

1  \begin{axis}[
    xlabel =
      Concentration\,/\/,\%
      mmol\,dm$^{-3}$,
5   xmax   = 400,
    xmin   = 0,
    ylabel = Rate\,/\/,s$^{-1}$,
    ymax   = 300,
    ymin   = 0
10  ]
    ...
  
```





Großer Datensatz

- Datenfile „data-set-two.txt“

```
1 Time a b c d
0 49 7 41 1.3
67 55 9 33 1.6
134 61 10 26 1.9
5 200 65 12 20 1.9
...
```



Großer Datensatz

- Datenfile „data-set-two.txt“

```
1 Time a b c d
0 49 7 41 1.3
67 55 9 33 1.6
134 61 10 26 1.9
5 200 65 12 20 1.9
...
```

- Einlesen des Datenfiles

```
1 \pgfplotstableread{data-set-two.txt}
\datatable
```

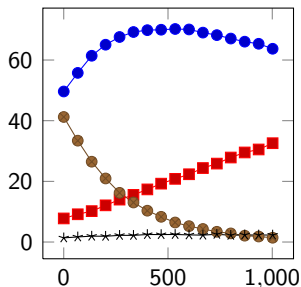
Großer Datensatz

■ Erzeugen des Plots

```

1 \pgfplotstableread{data-set-two.txt}
  \datatable

\addplot table[y = a] from \datatable ;
5 \addplot table[y = b] from \datatable ;
\addplot table[y = c] from \datatable ;
\addplot table[y = d] from \datatable ;
  
```



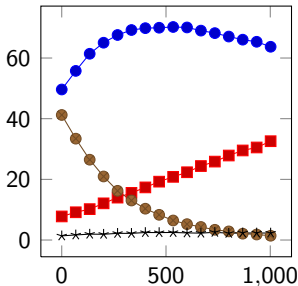
Großer Datensatz

■ Alternative

```
1 \pgfplotstableread{data-set-two.txt}
  \datatable
```

5

```
\addplot table[y = a] from \datatable ;
\addplot table[y = b] {data-set-two.txt} ;
10 \addplot table[y index = 3] {data-set-two.txt} ;
\addplot table[y index = 4] from \datatable ;
```

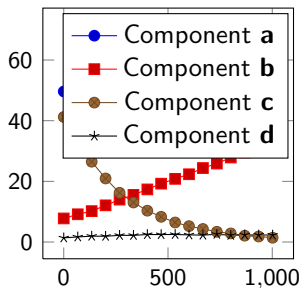


Großer Datensatz

■ Hinzufügen einer Legende

```

1 \addplot table[y = a] from \datatable ;
  \addplot table[y = b] from \datatable ;
  \addplot table[y = c] from \datatable ;
  \addplot table[y = d] from \datatable ;
5
  \legend{%
      Component \textbf{a},
      Component \textbf{b},
      Component \textbf{c},
10     Component \textbf{d},
  }
  
```



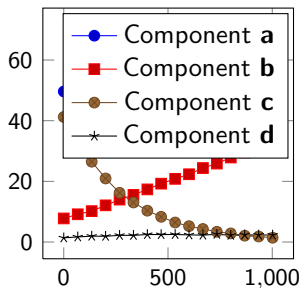
Großer Datensatz

Alternative

```

1 \begin{axis}[
    legend entries = {%
        Component \textbf{a},
        Component \textbf{b},
5     Component \textbf{c},
        Component \textbf{d},
    },
]

10 \addplot table[y = a] from \datatable ;
    \addplot table[y = b] from \datatable ;
    \addplot table[y = c] from \datatable ;
    \addplot table[y = d] from \datatable ;
  
```



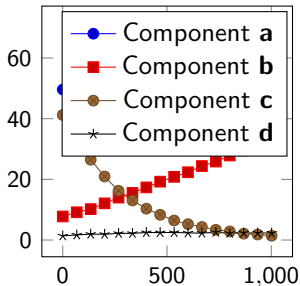
Großer Datensatz

- Noch eine Alternative

```

1 \addplot table[y = a] from \datatable ;
   \addlegendentry{%
     Component \textbf{a}};
\addplot table[y = b] from \datatable ;
5 \addlegendentry{%
   Component \textbf{b}};
...

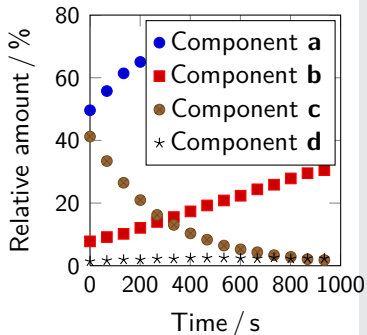
```



Großer Datensatz

- Schönheitskorrekturen
 - Achsenbeschriftungen hinzufügen
 - Linien entfernen
 - 1000er Trenner entfernen

```
1 \pgfkeys{  
  /pgf/number format/  
  set thousands separator =  
}
```



Großer Datensatz

- Eigene Marker definieren

```
1 \pgfdeclareplotmark{halfcircle}{%  
  \begin{pgfscope}  
    \pgfsetfillcolor{white}%  
    \pgfpathcircle{\pgfpoint{0pt}{0pt}}  
5    {\pgfplotmarksize}  
    \pgfusepathqfillstroke  
  \end{pgfscope}%  
  \pgfpathmoveto  
    {\pgfpoint{\pgfplotmarksize}{0pt}}  
10 \pgfpatharc{0}{180}{\pgfplotmarksize}  
  \pgfpathclose  
  \pgfusepathqfill  
}
```

- Ergebnis (200%)





Großer Datensatz

- neuen Marker verwenden

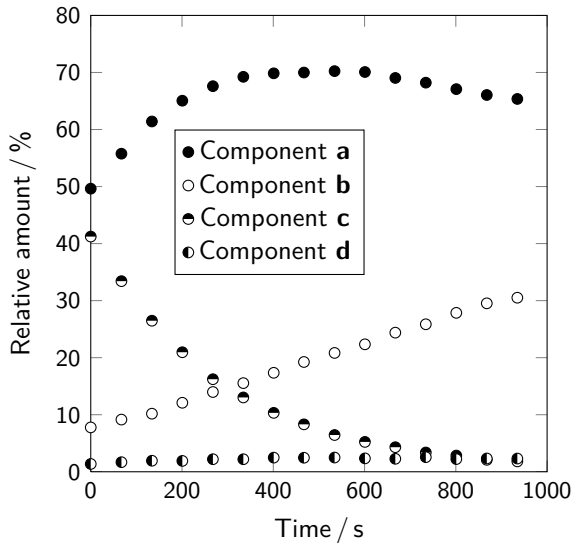
```
1 \addplot[mark = halfcircle, ...
```

- ... mit Optionen

```
1 \addplot[  
    mark           = halfcircle,  
    mark options = {rotate = 90},
```

- Legende verschieben

```
1 [  
    legend style = { at = {(0.6,0.75)}}  
]
```



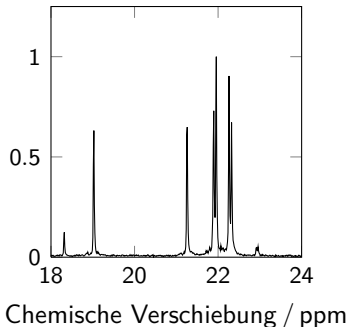
Ein experimentelles Spektrum

- was wir schon kennen

```

1  [
    xlabel = Chemische
      Verschiebung\,/\/,ppm,
    xmin   = 18,
    5      xmax   = 24,
    ymax   = 1.25,
    ymin   = 0
  ] \addplot[
    color = black,
    10     mark   = none
  ] table {plots/data/data-set-three.txt};

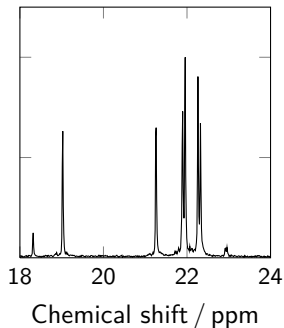
```



Ein experimentelles Spektrum

- y-Achsenbeschriftung entfernen

1 [yticklabels =]



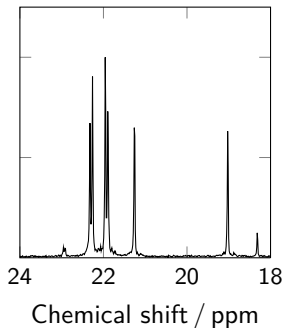
Ein experimentelles Spektrum

- y -Achsenbeschriftung entfernen

```
1 [yticklabels = ]
```

- x -Achse umdrehen

```
1 \addplot[
  x dir = reverse,
  ...
```



Ein experimentelles Spektrum

- Peaks beschriften

```
1 \node[  
  coordinate,  
  pin = {[rotate=90]right:22.26}  
] at (axis cs:22.26,1.1) { };
```



Ein experimentelles Spektrum

- Peaks beschriften

```
1 \node[
  coordinate,
  pin = {[rotate=90]right:22.26}
] at (axis cs:22.26,1.1) { };
```

22.26

- gedrehte Beschriftung

```
1 \node[
  coordinate,
  pin = {[rotate=90]5:22.32}
] at (axis cs:22.32,1.1) { };
```

22.32

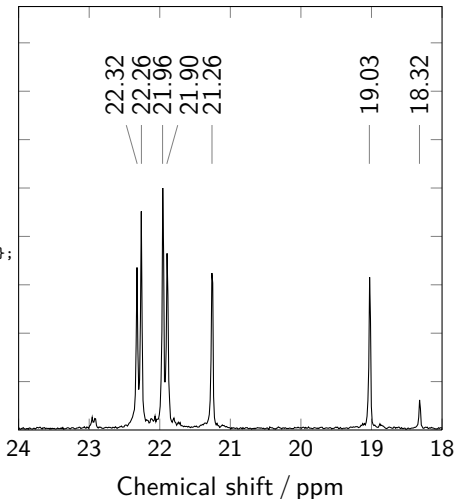
Ein experimentelles Spektrum

```

1  [
    x dir      = reverse,
    xlabel
= Chemical shift\,/,\,ppm,
    xmin      = 18,
5   xmax      = 24,
    ymax      = 1.75,
    ymin      = 0,
    yticklabels =
] \addplot[
10  color = black,
    mark = none
] table from {plots/data/data-set-three.txt};

\node[
15  coordinate,
    pin = {[rotate=90]5:22.32}
] at (axis cs:22.32,1.1) { }; \node[
    coordinate,
    pin = {[rotate=90]right:22.26}
20 ] at (axis cs:22.26,1.1) { }; ...

```





Funktionen mit GNUplot

- Formel

$$E(\Theta) = K \frac{(K \Theta)^{K-1}}{(K-1)!} \exp(-K \Theta)$$

Funktionen mit GNUplot

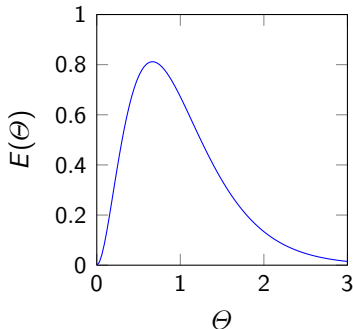
- Formel

$$E(\theta) = K \frac{(K \theta)^{K-1}}{(K-1)!} \exp(-K \theta)$$

```

1 % number of CSTRs
  \newcommand\K{3}

\addplot gnuplot[
5     id=cascade_model_full,
     domain=\xmin:\xmax,
     samples=101,
]
10     {\K * (\K*x)^(\K-1) / (\K-1)!
        * exp(-\K * x)};
  
```



- shell-escape nicht vergessen



Funktionen mit GNUplot

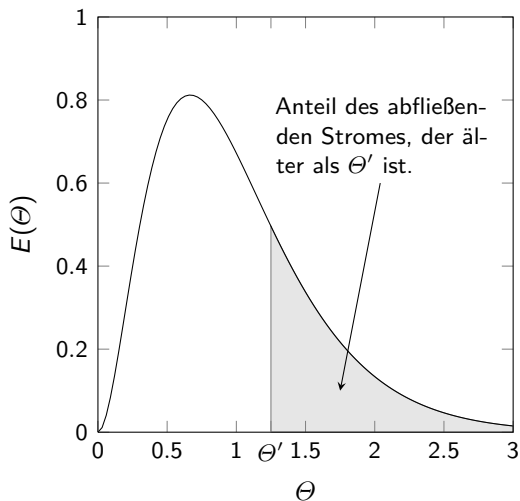
■ cascade_model_full.gnuplot

```
1 set table "cascade_model_full.table"; set format "%.5f"  
set format "%.7e";; set samples 101; set dummy x,y; plot [x=0:3] 3* (3
```

■ cascade_model_full.table

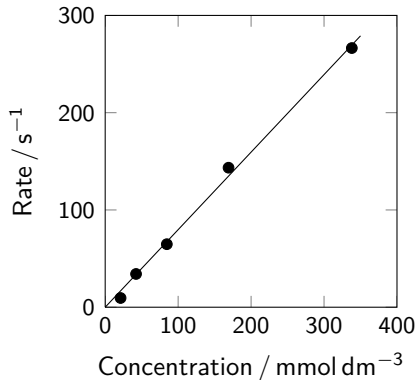
```
1  
# Curve 0 of 1, 101 points # Curve title: "3* (3*x)**(3-1) / (3-1)! *  
exp(-3* x)" # x y type 0.0000000e+000 0.0000000e+000 i 3.0000000e-002  
1.1104264e-002 i 6.0000000e-002 4.0594132e-002 i ...
```

Funktionen mit GNUplot



Berechnungen mit GNUplot (und Co.)

- erstes Beispiel noch einmal (Kleiner Datensatz)



Berechnungen mit GNUplot (und Co.)

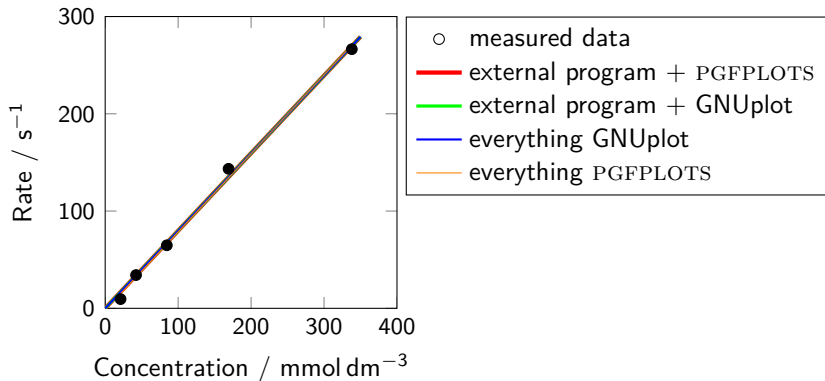
- erstes Beispiel noch einmal (Kleiner Datensatz)

1 ...

```
% plot regression curve with GNUplot (calculated also by GNUplot)
  \addplot [raw gnuplot] gnuplot [id=conc_rate] {
5   % define function which should be fitted
      f(x)=a*x;
   % let gnuplot fit using column 1 and 2 of the data file
      fit f(x) 'conc_rate.txt' using 1:2 via a;
   % Plot the function with the specified plot range
10  plot [x=\xmin:350] f(x); };
```


Berechnungen mit GNUplot (und Co.)

- erstes Beispiel noch einmal (Kleiner Datensatz)



Berechnungen mit GNUplot (und Co.)

- erstes Beispiel noch einmal (Kleiner Datensatz)

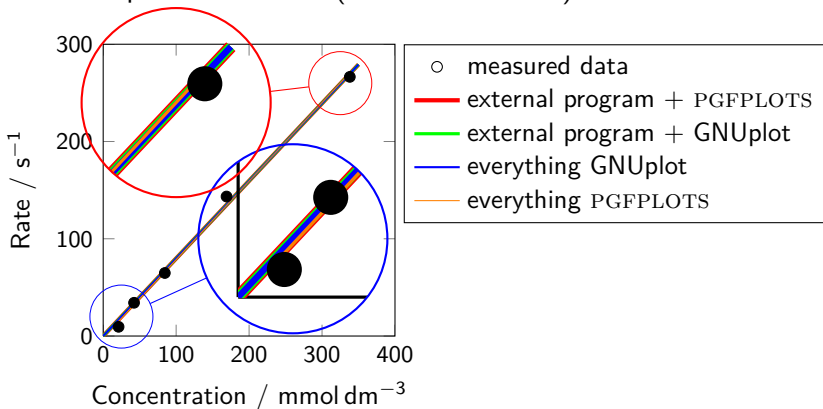




Diagramme exportieren

- nach PDF

```
1 \usetikzlibrary{pgfplots.external}  
   \tikzexternalize
```

- nach EPS

Diagramme exportieren

- nach PDF

```
1 \usetikzlibrary{pgfplots.external}  
   \tikzexternalize
```

- nach EPS

```
1 \tikzset{external/system call = {latex \tikzexternalcheckshellescape  
   -halt-on-error -interaction=batchmode -jobname "\image" "\texsource"  
   dvips -o "\image".ps "\image".dvi}}
```



Zusammenfassung

- pgfplots ist ein mächtiges Paket zum Erstellen von Diagrammen
- Die Diagramme sind
 - verschiedensten Typs (Linien, Balken, 2D, 3D, Dreieck)
 - hoher Qualität
 - konsistent zum restlichen Dokument
 - leicht anpassbar im Stil
- Keine Drittsoftware nötig

Literatur



J. Wright

Plotting experimental data using pgfplots

TUGboat 31:1, 2010, p. 50

[https:](https://www.tug.org/members/TUGboat/tb31-1/tb97wright-pgfplots.pdf)

[//www.tug.org/members/TUGboat/tb31-1/tb97wright-pgfplots.pdf](https://www.tug.org/members/TUGboat/tb31-1/tb97wright-pgfplots.pdf)



Chr. Feuersänger

PGFPLOTS manual

<http://pgfplots.sourceforge.net/pgfplots.pdf>

<http://pgfplots.sourceforge.net/pgfplotstable.pdf>



T. Tantau

PGF / TikZ manual

<http://sourceforge.net/projects/pgf>

