

Computer simulation of a time-of-flight mass spectrometer

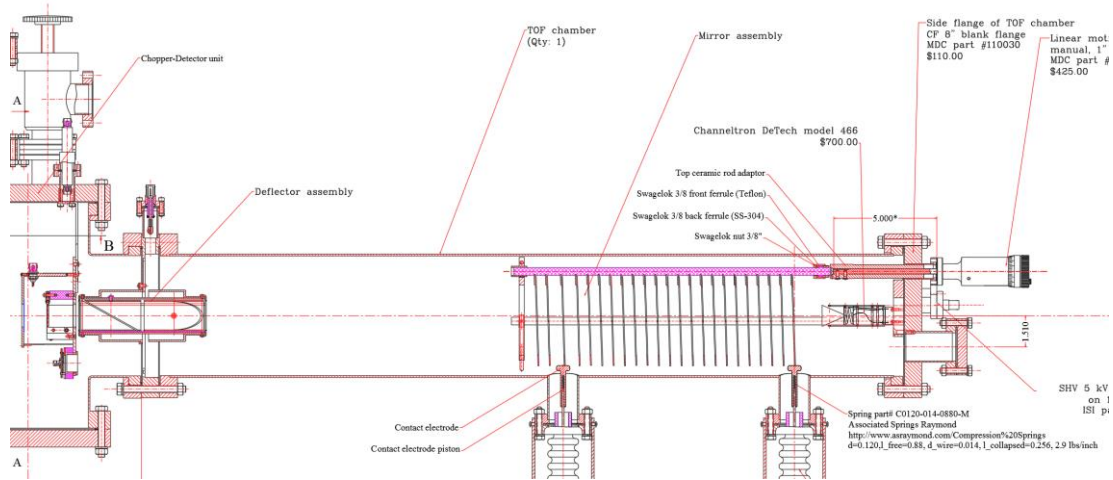
Leo Roeckenwagner, Svenja Benkert

Time-of-flight mass spectrometer



- Determining mass per charge ratio
- Ion source

Functional principle

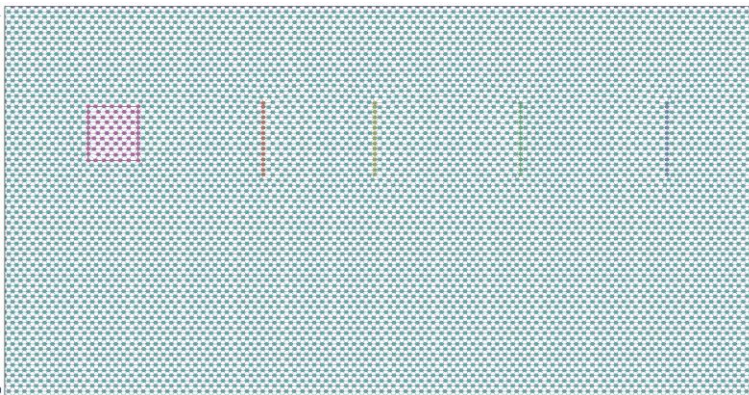


- Mass reflectron
- Ions are reflected by field of the mirror
- Measuring time of flight (tof)

Courtesy of A. Pikin

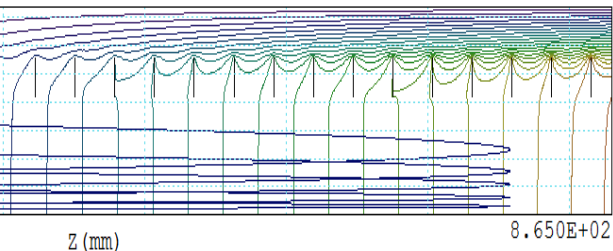
Our work - aim

- What are typical times of flight in this spectrometer?
- What resolution can we achieve with this spectrometer?
- What are the optimal settings?



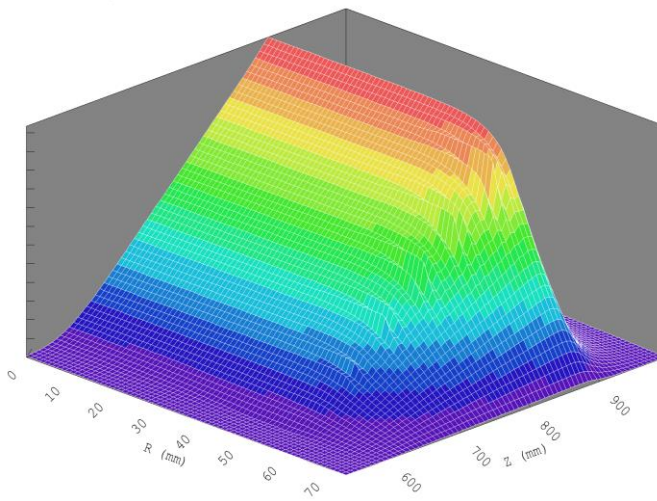
Mesh

Tracking particles



Analysis

Electrical field



```

PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
IndexError: 'ACCELERATING_VELOCITY', 'TIME_OF_FLIGHT', dtype='object')
Traceback (most recent call last):
  File "C:\Anaconda3\lib\site-packages\pandas\core\indexes\base.py", line 2657, in get_loc
    return self._engine.get_loc(key)
  File "pandas\libs\index.pyx", line 180, in pandas._libs.index.IndexEngine.get_loc
  File "pandas\libs\index.pyx", line 132, in pandas._libs.index.IndexEngine.get_loc
  File "pandas\libs\hashtable_class_helper.pxi", line 1601, in pandas._libs.hashtable.PyObjectHashTable.get_item
  File "pandas\libs\hashtable_class_helper.pxi", line 1608, in pandas._libs.hashtable.PyObjectHashTable.get_item
KeyError: 'TIME_OF_FLIGHT'

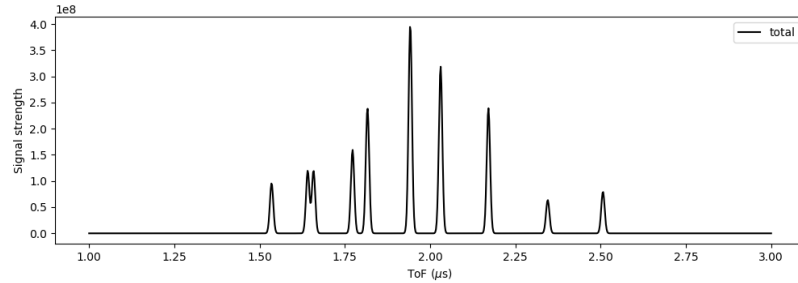
During handling of the above exception, another exception occurred:

Traceback (most recent call last):
  File ".\spektrum.py", line 7, in <module>
    plt.hist(df['TIME_OF_FLIGHT'])
  File "C:\Anaconda3\lib\site-packages\pandas\core\frame.py", line 2927, in _getitem_
    indexer = self.columns.get_loc(key)
  File "C:\Anaconda3\lib\site-packages\pandas\core\indexes\base.py", line 2659, in get_loc
    return self._engine.get_loc(self._maybe_cast_indexer(key))
  File "pandas\libs\index.pyx", line 180, in pandas._libs.index.IndexEngine.get_loc
  File "pandas\libs\index.pyx", line 132, in pandas._libs.index.IndexEngine.get_loc
  File "pandas\libs\hashtable_class_helper.pxi", line 1601, in pandas._libs.hashtable.PyObjectHashTable.get_item
  File "pandas\libs\hashtable_class_helper.pxi", line 1608, in pandas._libs.hashtable.PyObjectHashTable.get_item
KeyError: 'TIME_OF_FLIGHT'

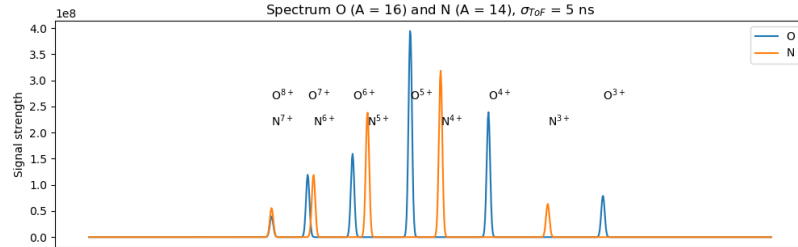
PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
IndexError: 'ACCELERATING_VELOCITY', 'TIME_OF_FLIGHT', dtype='object')
PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
Traceback (most recent call last):
  File ".\spektrum.py", line 7, in <module>
    bins = np.arange(1e-6, 12e-16, 1e-9)
NameError: name 'np' is not defined
PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
Traceback (most recent call last):
  File ".\spektrum.py", line 10, in <module>
    plt.hist(df[' TIME_OF_FLIGHT'], bins)
  File "C:\Anaconda3\lib\site-packages\matplotlib\pyplot.py", line 2659, in hist
    **({"data": data} if data is not None else {}), **kwargs)
  File "C:\Anaconda3\lib\site-packages\matplotlib\axes\_axes.py", line 1818, in inner
    return func(*args, **kwargs)
  File "C:\Anaconda3\lib\site-packages\matplotlib\axes\_axes.py", line 6594, in hist
    mlist = np.zeros(len(bins)-1, m.dtype)
ValueError: negative dimensions are not allowed
PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
QObject::QObject: Timers cannot be stopped from another thread
PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
C:\Anaconda3\lib\site-packages\scipy\stats\stats.py:1713: FutureWarning: Using a non-tuple sequence for multidimensional indexing is deprecated; use `arr[tuple(seq)]` instead of `arr[seq]`. In the future this will be interpreted as an array index, `arr[np.array(seq)]`, which will result either in an error or a different result.
    return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
C:\Anaconda3\lib\site-packages\scipy\stats\stats.py:1713: FutureWarning: Using a non-tuple sequence for multidimensional indexing is deprecated; use `arr[tuple(seq)]` instead of `arr[seq]`. In the future this will be interpreted as an array index, `arr[np.array(seq)]`, which will result either in an error or a different result.
    return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
PS C:\VOPSIM\tofsim_05_15_2019> python .\spektrum.py
PS C:\VOPSIM\tofsim_05_15_2019> python .\plotting/energyfocus.py
fortrl: error (200): program aborting due to control-c event
Image          PC          Routine          Line          Source
libifcoremd.dll 000077FB545900C4 Unknown          Unknown       Unknown
KERNELBASE.dll 000077FC5F997223 Unknown          Unknown       Unknown
KERNEL32.DLL 000077FC633384D4 Unknown          Unknown       Unknown
ntdll.dll       000077FC635B8E51 Unknown          Unknown       Unknown
QObject::QObject: Timers cannot be stopped from another thread
PS C:\VOPSIM\tofsim_05_15_2019> python .\plotting/energyfocus.py
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ntdll.dll       000077FC635B8E51 Unknown          Unknown       Unknown
QObject::QObject: Timers cannot be stopped from another thread
PS C:\VOPSIM\tofsim_05_15_2019> python .\plotting/energyfocus.py
PS C:\VOPSIM\tofsim_05_15_2019> []
  
```



Typical times of flight



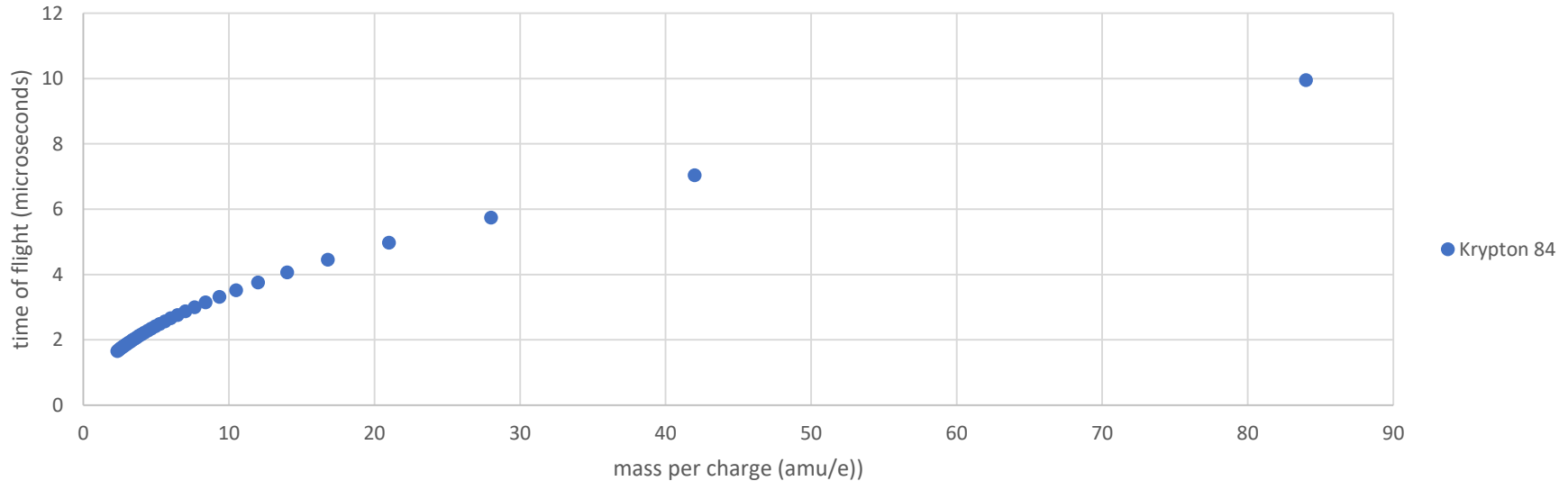
Overlapping spectrum



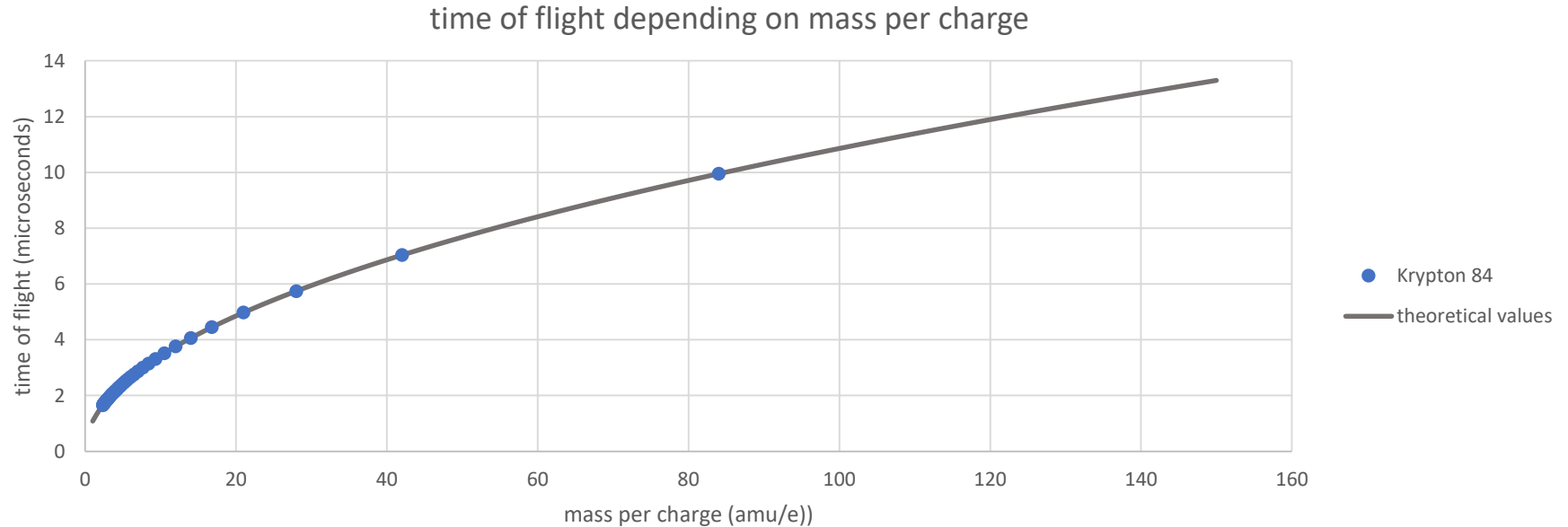
Individual spectrums

Theoretical and simulation values

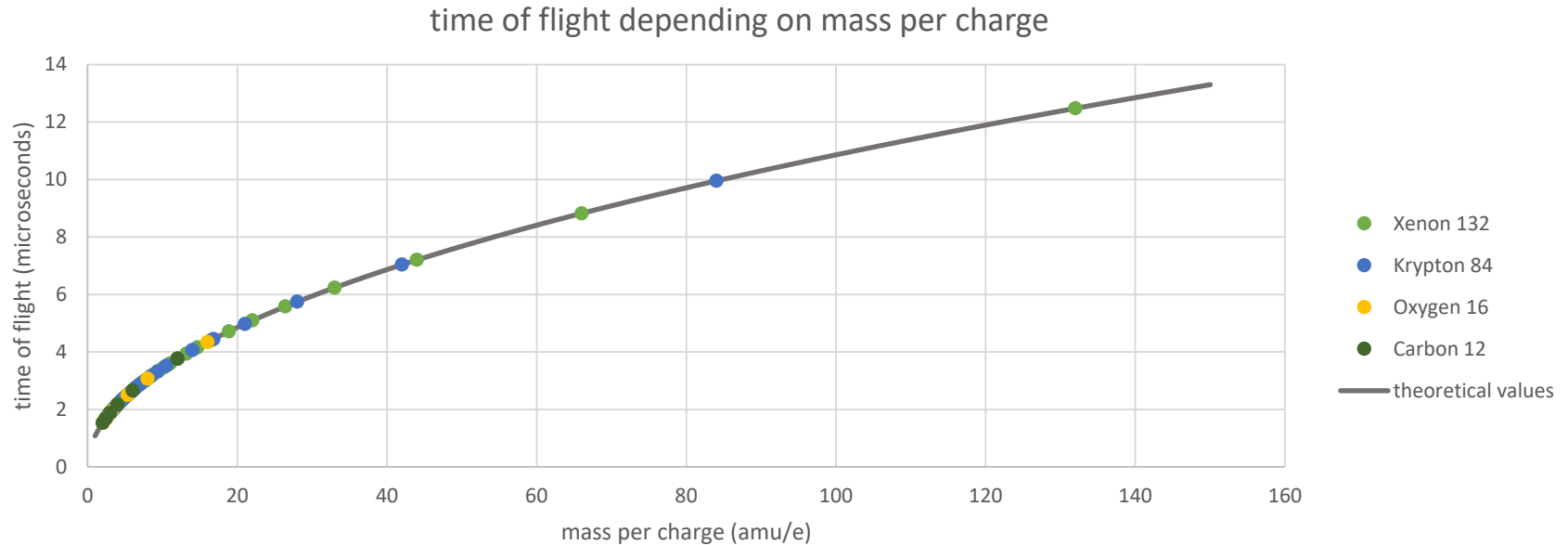
time of flight depending on mass per charge



Theoretical and simulation values

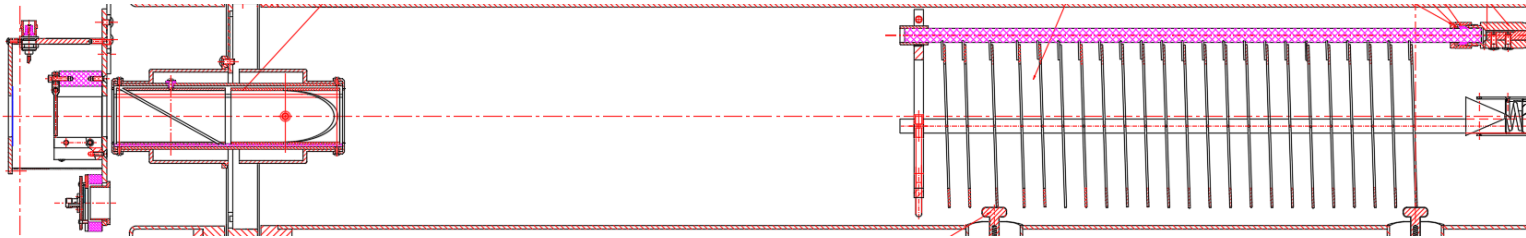


Theoretical and simulation values



Theoretical model

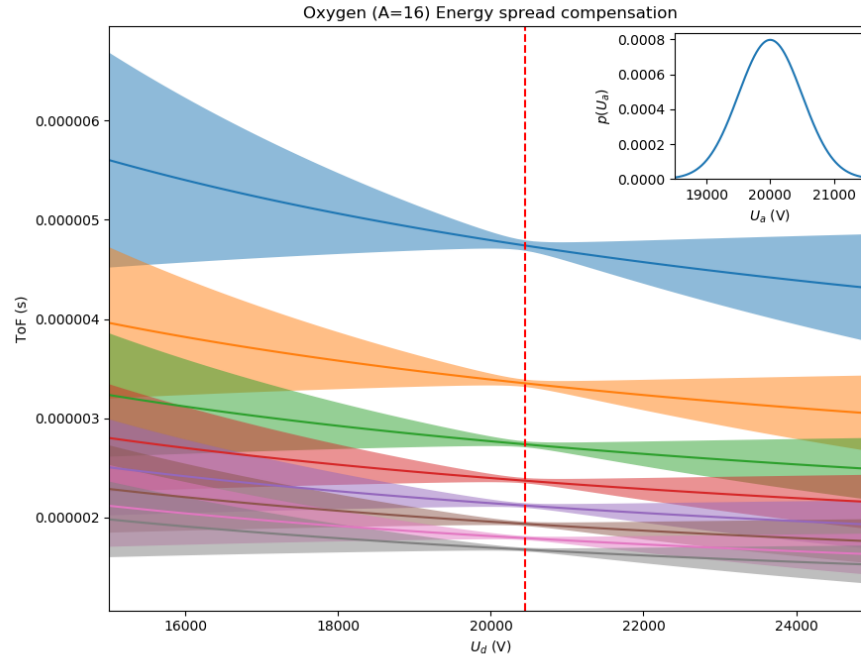
$$\Delta t = 2 \sqrt{\frac{m}{q}} \left(\frac{s}{\sqrt{2U}} + \frac{\sqrt{2U}}{E_d} \right)$$



Our work - aim

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- What resolution can we achieve with this spectrometer?
- **What are the optimal settings?**

Energy spread - optimization



THANK YOU!!!

Any questions?

With special thanks to Hannes Pahl