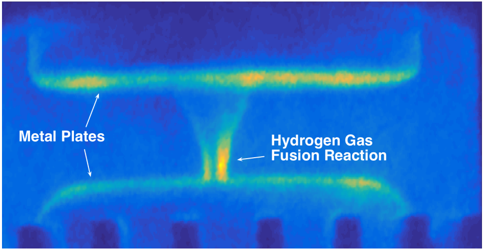
DOE/NV/25946--2379

An MCMC Approach to Quantifying Reaction Uncertainties in Controlled Fusion

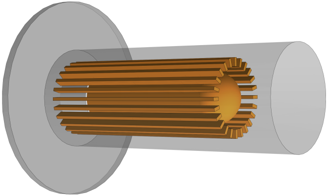


Aaron Luttman
Principal Scientist (Mathematician)
Defense Experimentation and Stockpile Stewardship
National Security Technologies, LLC

Joint work with the NSTec Dense Plasma Focus Research Group

This work was done by National Security Technologies, LLC, under Contract No. DE-AC52-06NA25946 with the U.S. Department of Energy and supported by the Site-Directed Research and Development Program.

Neutron Time of Flight



Primary Problem: Determine the creation time and energy characteristics for neutrons generated in a controlled fusion reaction.

Dense Plasma Focus (DPF):
Deuterium or Deuterium and Tritium get fully ionized to form a plasma then get compressed to the point of fusing, emitting photons and neutrons.

Radiation Detectors

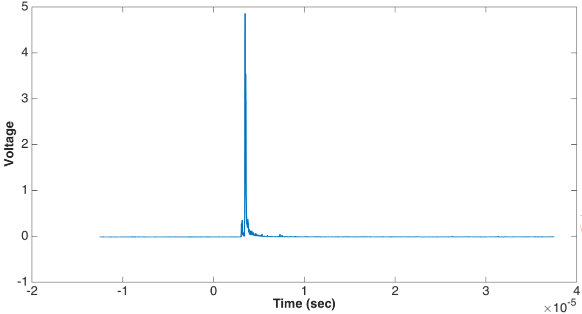
Neutron Detectors:

1. Neutron interacts with scintillator, which releases a charged particle,
2. which bounces around and releases photons,
3. into a photomultiplier tube.
4. Released photons hit the photocathode,
5. generating a flow of electrons.

Notes:

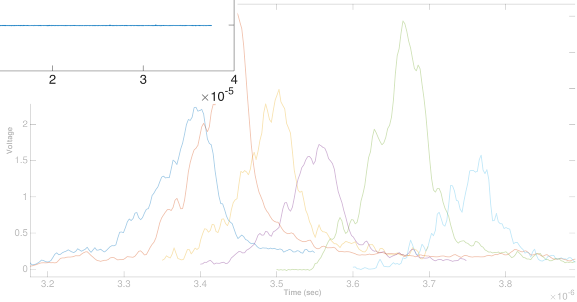
- Neutrons are counted without regard to energy.
- Neutrons have mass, so higher energy neutrons are faster than low energy neutrons.
- Scatter effects are difficult to distinguish from the desired interactions.

Detector Signals



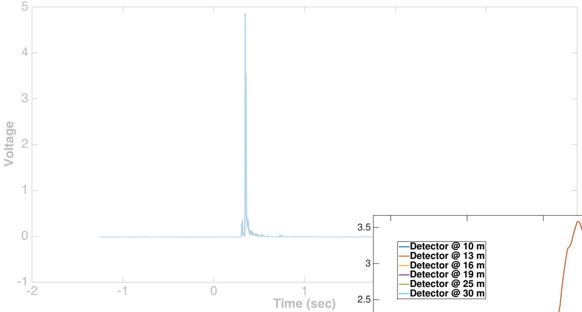
Signal is from shot 3 on November 20, 2014.

Detector at 25 m.



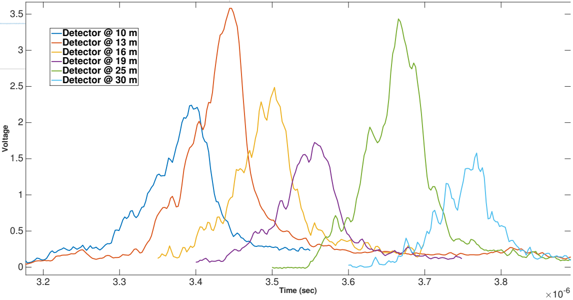
Signals are from shot 8 on November 19, 2014.

Detector Signals



Signal is from shot 3 on November 20, 2014.

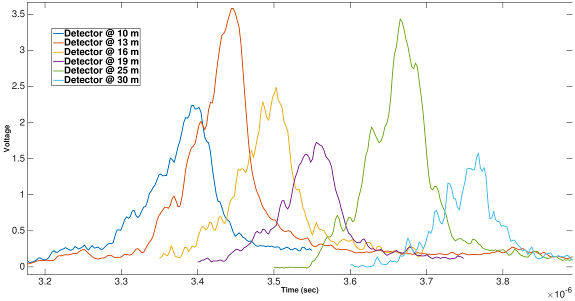
Detector at 25 m.



Signals are from shot 8 on November 19, 2014.

Time of Flight

KEY FEATURE: Since neutrons have mass, neutrons of different energies travel at different speeds. Thus, the neutron detector signals broaden as a function of distance from the detector.



Signals are from shot 8 on November 19, 2014.

Mathematical Formulation

The neutron time of flight (NToF) model for the measurement at a detector is

$$S(X,t') = \frac{\kappa N \alpha A}{4\pi X^2} \int_0^\infty \int_{-\infty}^\infty F(v,t)\delta\left(t - \left(t' - \frac{X}{v}\right)\right) dt\, dv$$
$$= \frac{\kappa N \alpha A}{4\pi X^2} \int_0^\infty F\left(v, t' - \frac{X}{v}\right) dv,$$

where

- t – Neutron creation time,
- t' – Neutron detection time,
- X – Distance from source to detector,
- v – Neutron velocity,
- F – Neutron time-velocity spectrum at creation,
- N – Total neutron yield
- α – Detector efficiency, and
- A – Detector surface area

Mathematical Formulation

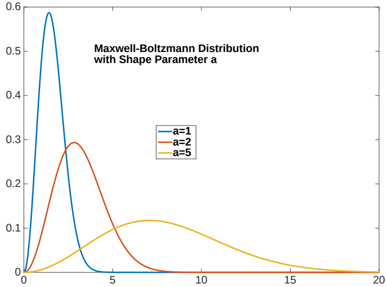
The neutron time of flight (NToF) model for the measurement at a detector is

$$
\begin{aligned}
S(X, t') &= \frac{\kappa N \alpha A}{4\pi X^2} \int_0^\infty \int_{-\infty}^\infty F(v, t)\delta\left(t - \left(t' - \frac{X}{v}\right)\right) dt\, dv \\
&= \frac{\kappa N \alpha A}{4\pi X^2} \int_0^\infty F\left(v, t' - \frac{X}{v}\right) dv,
\end{aligned}
$$

where

- t – Neutron creation time,
- t' – Neutron detection time,
- X – Distance from source to detector,
- v – Neutron velocity,
- F – Neutron time-velocity spectrum at creation,
- N – Total neutron yield
- α – Detector efficiency, and
- A – Detector surface area

Reaction Model



Assuming a Maxwell-Boltzmann distribution for neutron creation time and a Gaussian distribution in energy,

$$f_1(v) = \frac{2v}{\sqrt{2\pi}\sigma_E} \exp\left(\frac{-(v^2 - E_0)^2}{2\sigma_E^2}\right)$$

$$f_2(t) = \sqrt{\frac{2}{\pi}} \frac{(t - t_0)^2 \exp\left(\frac{-(t-t_0)^2}{2a_t^2}\right)}{a_t^3}$$

and a separable total number distribution gives

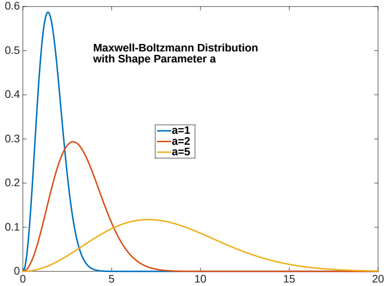
$$F(v,t) = f_1(v)f_2(t) = \frac{2v(t - t_0)^2}{\pi\sigma_E a_t^3} \exp\left(-\frac{(v^2 - E_0)^2}{2\sigma_E^2} - \frac{(t - t_0)^2}{2a_t^2}\right)$$

Reaction Model

Assuming a Maxwell-Boltzmann distribution for neutron creation time and a Gaussian distribution in energy,

$$f_1(v) = \frac{2v}{\sqrt{2\pi}\sigma_E} \exp\left(\frac{-(v^2 - E_0)^2}{2\sigma_E^2}\right)$$

$$f_2(t) = \sqrt{\frac{2}{\pi}} \frac{(t-t_0)^2 \exp\left(\frac{-(t-t_0)^2}{2a_t^2}\right)}{a_t^3}$$



and a separable total number distribution gives

$$F(v,t) = f_1(v) f_2(t) = \frac{2v(t-t_0)^2}{\pi\sigma_E a_t^3} \exp\left(-\frac{(v^2 - E_0)^2}{2\sigma_E^2} - \frac{(t-t_0)^2}{2a_t^2}\right)$$

E_0 is the peak energy; σ_E is the energy spread; t_0 is initial neutron creation time; and a_t is a time profile shape parameter.

Parametric Inverse Problem

Thus the goal is to compute the optimal model parameters

$$\theta = \{t_0, v_0, a_t, a_v, \kappa_1, \ldots, \kappa_M\}$$

from

$$\begin{aligned} b_j := S(X_j, t') &= \frac{\kappa_j N \alpha A}{4\pi X_j^2} \int_0^\infty F\left(v, t' - \frac{X_j}{v}\right) dv \\ &= \frac{\kappa_j N \alpha A}{2\pi^2 X_j^2 \sigma_E a_t^3} \int_0^\infty (v(t' - t_0) - X) \exp\left(-\frac{(v^2 - E_0)^2}{2\sigma_E^2} - \frac{(v(t' - t_0) - X)^2}{2v^2 a_t^2}\right) dv, \\ &:= T(X_j, t', N, \alpha, A, \theta) \end{aligned}$$

given the measurements from detectors at distances $\{X_1, X_2, \ldots, X_M\}$.

Statistical Formulation

The Bayesian formulation for solving the associated least squares problem is

$$p(b|\theta) \propto \exp\left(-\frac{1}{2}\sum_{j=1}^{M}\|b_j - T(X_j, t', N, \alpha, A, \theta)\|^2\right).$$

We place a Gaussian prior on θ,

$$p(\theta) \propto \exp\left(-\theta^T C^{-1}\theta\right),$$

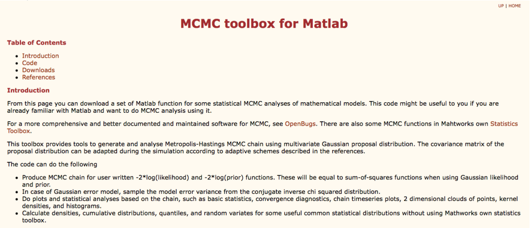
where C is the parameters' covariance, which gives the posterior

$$p(\theta|b) \propto \exp\left(-\frac{1}{2}\sum_{j=1}^{M}\|b_j - T(X_j, t', N, \alpha, A, \theta)\|^2 - \theta^T C^{-1}\theta\right).$$

MCMC Toolbox*

In order to compute the optimal parameter values, we sample from the posterior using a Markov Chain Monte Carlo approach.

```
%   This just sets up the parameters structure, based on the input above.
Params = {
           %      name,    init,                                     min,      max,   mu,   sig, target?, local?
              {'kappa', 3500*ones(NumDetectors,1),  zeros(NumDetectors,1),   1e6*ones(NumDetectors,1),  NaN,  Inf,   1,      1}
              {'t0',    7400,                                     -10000,   8200,  NaN,  Inf,   1,      0}
              {'v0',       0,                                          0,      10,  NaN,  Inf,   1,      0}
              {'av',       1,                                          0,      10,  NaN,  Inf,   1,      0}
              {'at',       1,                                          0,      10,  NaN,  Inf,   1,      0}
              {'alpha',    alpha*ones(NumDetectors,1),                 0,       0,  NaN,  Inf,   0,      1}
              {'A' ,       Area*ones(NumDetectors,1),                  0,       0,  NaN,  Inf,   0,      1}
              {'N',        NeutronYield,                               0,       0,  NaN,  Inf,   0,      1}
              {'X',        X,                                          0,       0,  NaN,  Inf,   0,      1}
                 };
```


UP | HOME

MCMC toolbox for Matlab

Table of Contents

Introduction

From this page you can download a set of Matlab function for some statistical MCMC analyses of mathematical models. This code might be useful to you if you are already familiar with Matlab and want to do MCMC analysis using it.

For a more comprehensive and better documented and maintained software for MCMC, see OpenBugs. There are also some MCMC functions in Mahtworks own Statistics Toolbox.

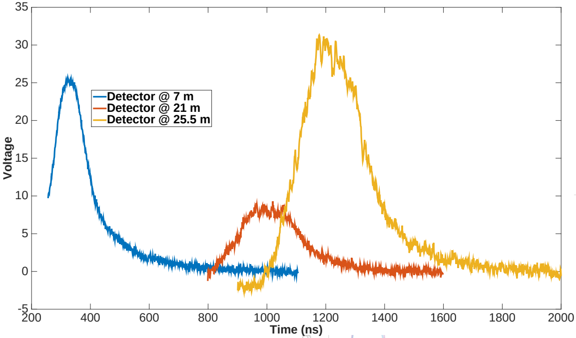
This toolbox provides tools to generate and analyse Metropolis-Hastings MCMC chain using multivariate Gaussian proposal distribution. The covariance matrix of the proposal distribution can be adapted during the simulation according to adaptive schemes described in the references.

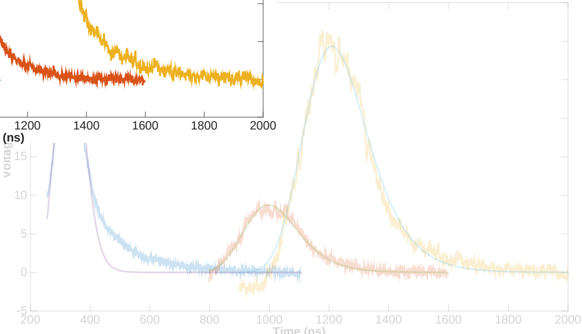
The code can do the following

- Produce MCMC chain for user written -2*log(likelihood) and -2*log(prior) functions. These will be equal to sum-of-squares functions when using Gaussian likelihood and prior.
- In case of Gaussian error model, sample the model error variance from the conjugate inverse chi squared distribution.
- Do plots and statistical analyses based on the chain, such as basic statistics, convergence diagnostics, chain timeseries plots, 2 dimensional clouds of points, kernel densities, and histograms.
- Calculate densities, cumulative distributions, quantiles, and random variates for some useful common statistical distributions without using Mathworks own statistics toolbox.

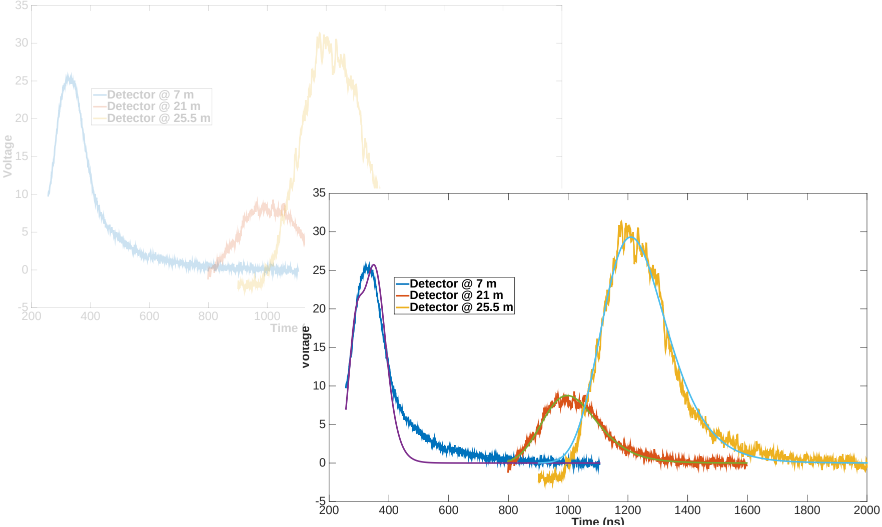
* H. Haario, M. Laine, A. Mira and E. Saksman, 2006. "DRAM: Efficient adaptive MCMC," *Statistics and Computing*, **16** (2006), pp. 339-354. (doi:10.1007/s11222-006-9438-0)

D-D Results

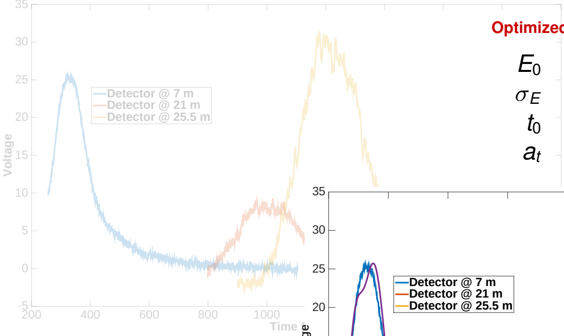




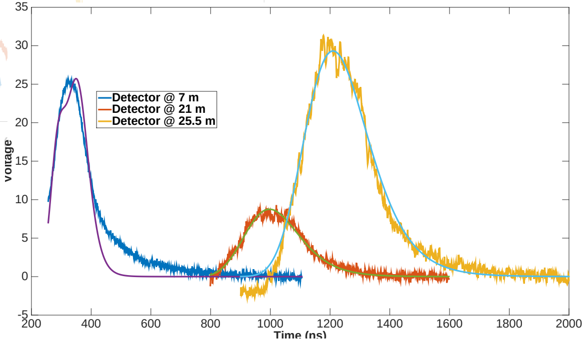
D-D Results


Detector @ 7 m
Detector @ 21 m
Detector @ 25.5 m
voltage
Time (ns)
35
30
25
20
15
10
5
0
-5
200
400
600
800
1000
1200
1400
1600
1800
2000

D-D Results



Optimized Parameters			95% credible intervals
E_0	=	2.219	(2.213, 2.224)
σ_E	=	0.391	(.388, .394)
t_0	=	-5.74	$(-6.68, -4.78)$
a_t	=	20.31	(20.01, 20.63)



Thanks!

Feel free to email me at

luttmaab@nv.doe.gov

with questions, comments, or for offprints/preprints.