Markov chain Monte Carlo (MCMC) with parallel tempering to calibrate Gaia's radiation damage model

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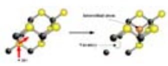
Abstract

With its 106 CCD image sensors, the Gaia mission aims to create a complete and highly accurate stereoscopic map of the Milky Way. The performance of CCDs is degraded in space by the effect of solar radiation which reduces the high charge transfer efficiency through charge trapping. This effect implies for Gaia a charge loss and a centroid bias which reduce the accuracy of the measurements. A large effort has been devoted to characterize and mitigate this effect as much as possible through large ground test campaigns and simulations.

A Charge Distortion Model (CDM) is used within the Gaia community to quantify the impact of radiation on measurements. The determination of the CDM parameters from a fit to experimental data requires a global approach as the distribution of the parameters for the modeling displays many local minima. An experimental Java implementation of MCMC with parallel tempering has been developed to determine the parameters of the CDM. This tool is described and some results are presented in the case of data impacted by the trapping occurring in the CCDs serial register.

Radiation Damage: Traps & CTI

The displacement of atoms in the silicon lattice of the Gaia CCDs by solar flare protons will result in the creation of defects (vacancies, V). They can wander through the lattice to locations where they can form stable complexes which introduce localized energy levels within the band gap of the semiconductor. These energy levels trap the signal carriers (electrons here) and increase the charge transfer inefficiency (CTI). Depending on the type of complex (P-V, V-V, etc.), different "trap species" are created.



Non-ionizing or displacement damage: incident radiation interacts directly with the atomic nucleus with enough energy to displace the atoms from their positions in the crystal lattice.

The stochastic capture and release by the traps of the charges result in a significant charge loss and distortion of the stellar image. Charge loss and distortion ...
... change with trap occupancies.
... are different in different areas of the CCD.
... worsen during the mission.
Radiation damage of the Gaia CCDs is impacting centroiding and flux determination[1].

A Charge Distortion Model (CDM)

A fast analytical model of the CTI effects has been developed to realistically reproduce the radiation damage whilst still being computationally inexpensive for use in the Gaia data processing pipeline. The model is based on the common Shockley-Read-Hall formalism which describes the capture and release of a charge by an individual trap as a decay process with an associated time constant. However, **the CDM model treats all the traps of a species in statistical way[2].**

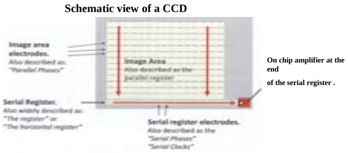
Tools for CDM calibration

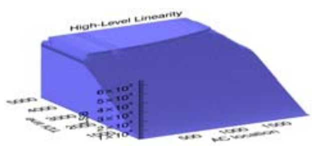
The CDM is a semi-empirical method and the trap parameters can be degenerated When fitting the model to test data, the likelihood displays many local maxima.
Consequently, a reasonable fit can be obtained from different set of parameters and does not necessarily produce parameters which have a physical meaning. Trying local methods like downhill simplex does not always work. A **global method** had to be chosen like MCMC with parallel tempering which offers, as a Bayesian method, much flexibility to constrain the parameters with priors.

The calibration data set

As in the image area, pixels in CCD serial register (SR hereafter) can potentially trap electrons from the signal. This trapping distorts the signal along the across scan direction..

Schematic view of a CCD





The test set up consists in a flat field illumination repeated for each transfer in the parallel direction. Consequently, the data set displays a level monotonically increasing in the parallel direction away from SR and **a trailing signal in the serial direction** from the over scanned pixels of the SR. The signal in the over scanned pixels is coming from the release of electrons by traps in the serial register. The CDM is expected to model the deferred charge in the trailing signal.

Bayesian estimation of CDM parameters

We want to estimate the CDM parameters from statistical inference. From Bayes' theorem, we have:

$$p(X \mid D, I) = \frac{p(X \mid I)\, p(D \mid X, I)}{p(D \mid I)}$$

p(X|D,I) is the posterior we want to sample. In our case, X is the vector of parameters corresponding to CDM[2]

- Trap species 1: Number of traps, release time constant, capture cross section.
- Trap species 2: Number of traps, release time constant, capture cross section.
- A coefficient describing electron cloud growth parameter: β_e (not to be confused with parallel tempering parameter).

p(D|X,I) is the likelihood.

- Gaussian model (convolution of a Poisson distribution for electron noise with normal distribution for readout noise).
- Gives the probability of having the simulated points far from the data points.

p(X|I) is the parameters prior. In the present case, only flat priors have been considered.

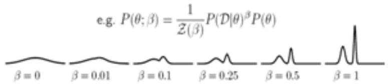
MCMC with parallel tempering

Markov Chain Monte Carlo methods are a class of algorithms for sampling from probability distributions based on constructing a Markov chain that has the desired distribution as its equilibrium distribution. The state of the chain after a large number of steps is then used as a sample of the desired distribution. Metropolis-Hastings algorithm is used as transition kernel.

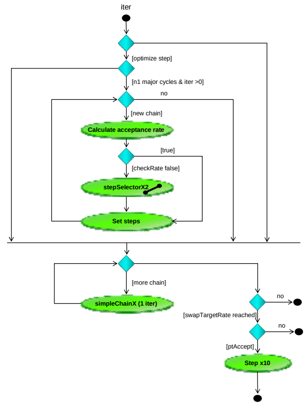
Parallel tempering

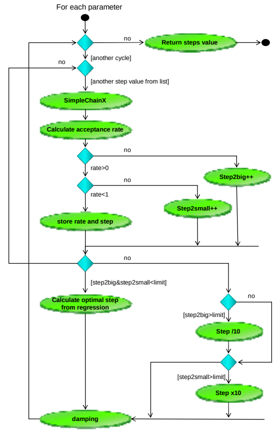
Multiple copies of the simulation are run in parallel, each with a tempering parameter β from a discrete set of values **{β_0, β_1,..., 1}**. The tempering parameter flattens the distribution and allows the potential exploration of all the modes. At intervals, a pair of adjacent chains, on the tempering parameter set, are chosen at random and a proposal is made to swap their parameter states. If accept, the swap allows for an exchange of information across the chains. The chain with β =1 is the desired target probability distribution. If β is defined as β =1/T, with T being a temperature, the method has a strong analogy with simulated annealing.

e.g. $P(\theta;\beta) = \frac{1}{Z(\beta)} P(\mathcal{D}|\theta)^{\beta} P(\theta)$



A versatile Java implementation[3]





Validation with synthetic data

The CDM parameter estimation of synthetic data was performed successfully starting from a realistic set of parameters derived from previous work. It can be noted that the 2 trap species have swapped their parameters which shows that the samples have wandered far from their initial value and gives confidence in the efficiency of the algorithm.

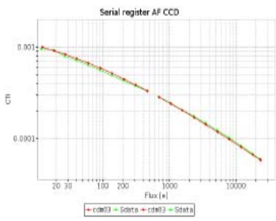
	Trap species 1			Trap species 2			
Parameters unit	Density [m^{-3}]	Rtc [s]	σ [m^{-2}]	Density [m^{-3}]	Rtc [s]	σ [m^{-2}]	β_e
simulated	3.11×10^{16}	1.1×10^{-7}	8.5×10^{-12}	1.33×10^{16}	5.5×10^{-7}	3.7×10^{-14}	0.300
starting	3.11×10^{16}	1.1×10^{-6}	8.5×10^{-12}	1.33×10^{16}	5.5×10^{-7}	3.7×10^{-14}	0.300
Output median	1.28×10^{16}	4.82×10^{-7}	6.15×10^{-11}	3.01×10^{16}	1.19×10^{-7}	5.53×10^{-13}	0.301
Output MAP	1.32×10^{16}	[illegible]3×10^{-7}	9.93×10^{-12}	2.95×10^{16}	1.18×10^{-7}	4.91×10^{-13}	0.303

Number of iterations	70,000
Number of chains	14
Target acceptance rate	20%
Target swapping rate	50%

Results

The parameter estimation has been applied to a real data set. The set of estimated parameters allow the model to fit the trailing curve reasonably well for all signal levels. The CTI curve is a positive quality check of the fit.

trails



CTI curve

Number of iterations	100,000
Number of chains	14
Target acceptance rate	20%
Target swapping rate	50%

Conclusion

A Java implementation of MCMC with parallel tempering has been developed. With this implementation, it was possible to calibrate CDM with a reasonable accuracy. Despite the complexity of its tuning, this implementation is versatile enough to be used for more general parameter estimations.

Acknowledgments

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