Simulations of Silicon Radiation Detectors for HEP

Benjamin Nachman (editor),[1] **Timo Peltola (editor),**[2] **F.R.Palomo,**[3] **Jory Sonneveld,**[4] **R. Lipton,**[5] **Patrick Asenov,**[6,7] **and add yourself**

[1] *Physics Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

[2] *Department of Physics and Astronomy, Texas Tech University, 1200 Memorial Circle, Lubbock, USA*

[3] *Electronic Engineering Dept., School of Engineering, University of Sevilla, 41092 Spain*

[4] *Nikhef National Institute for Subatomic Physics, Science Park 105, 1098 XG Amsterdam, Netherlands*

[5] *Fermilab, P.O. Box 500, Batavia Il USA*

[6] *INFN Sezione di Perugia, Perugia, Italy*

[7] *Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, Perugia, Italy*

E-mail: bpnachman@lbl.gov

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Should reference the recent Yellow Report [1].

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3.1 Models for Single Quantities

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3.2 TCAD Simulations for Detector Properties

Many multi-trap models for radiation damage and lighter-weight alternatives (TRACS and Weightfield2)

Radiation levels above $\sim 10^{13}$ $\mathrm{n_{eq}cm^{-2}}$ introduce observable damage to the crystal structure of a silicon sensor. Fluences beyond 1×10^{14} $\mathrm{n_{eq}cm^{-2}}$ lead eventually to a significant degradation of the detector performance. In the immense radiation environment of the HL-LHC, defects are introduced both in the silicon substrate (bulk or displacement damage) and in the SiO_2 passivation layer, that affect the sensor performance via the interface with the silicon (surface damage). The multitude of observed defect levels after irradiations with hadrons or higher energy leptons [2], set up a broad parameter space that is not practical to model and tune. Thus, minimized set of defects constituting various effective defect models have been applied as the approach for the simulations of irradiated silicon detectors. Most of these defect models have been developed for the professional finite-element TCAD[1] software frameworks Synopsys Sentaurus™[2] and Silvaco Atlas™[3].

The modeling of the main macroscopic effects of the bulk damage on high-resistivity Si-sensors irradiated by hadrons −the change of the effective doping concentration N_{eff} (resulting in modified electric field distribution), the increase in the leakage current proportional to the fluence and the degradation of charge collection efficiency (CCE)− includes two-level [3–7] and three-level models [8–10]. Figure 3 demonstrates a comparison between measured transient signals (Figure 3a) and CCE (Figure 3b) of neutron irradiated sensors and simulated results produced by a two-level defect model for neutrons.

Simulating the effects of the surface damage on Si/SiO_2-interface irradiated by charged hadrons, gammas or X-rays −like change of inter-electrode resistance (R_{int}) and capacitance (C_{int}), modified electric fields at implant edges and charge-injection position dependence of CCE− involves approaches, where surface damage is approximated solely by the fixed oxide charge density (N_{f}) [11–13] or by three interface traps (N_{it}) with parameters matching the measurements of X-ray irradiated MOS-capacitors [14]. Results from a further model that

[1] Technology Computer-Aided Design
[2] http://www.synopsys.com
[3] http://www.silvaco.com

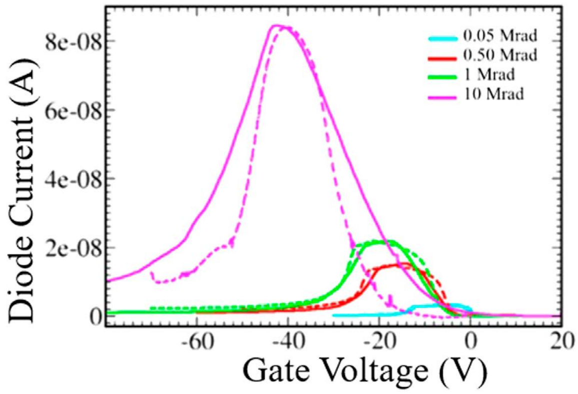


Figure 1. — I-V characteristics of n-on-p HPK gated-diode: comparison between the measured and simulated diode current as a function of gate voltage (with p-spray isolation layer). Measurements in solid line and simulations in dashed line. The model used in the simulation is "Perugia 2019 Surface".

combines the two approaches is presented in Figure 4, where the characteristics of the CV-curves of a γ-irradiated MOS-capacitor are only reproduced by simulation by including in addition to N_f both acceptor and donor-type deep N_it ($N_\mathrm{it,acc,don}$) at the Si/SiO$_2$-interface (Figure 4a). By using both N_f and $N_\mathrm{it,acc,don}$ as an input for an R_int-simulation with typical HGCAL[4] isolation implant parameters in Figure 4b, the experimentally observed R_int-values are quantitatively reproduced (atoll and common p-stops with STD N_ps). By excluding $N_\mathrm{it,acc,don}$ from the simulation, the pads become either shorted (STD N_ps, $N_\mathrm{it} = 0$) for all voltages or reach isolation only above 500 V of reverse bias voltage for an extreme value of p-stop peak doping ($5 \times$ STD N_ps, $N_\mathrm{it} = 0$).

First steps towards unified bulk and surface defect models include approach, where two bulk defect levels are augmented by an acceptor-type N_it with 2 μm depth distribution from the surface (Sentaurus [15–17]), and by a model where two bulk defect levels are complemented by two acceptor-type N_it (Atlas [18]). Details of the development of the defect models are described in e.g. [19].

3.2.1 Simulations of Large-Mesh Devices

In Synopsys Sentaurus TCAD software framework, the device structures can be generated in both 2D or 3D. Sensors that have negligible contribution to the weighting field from the third dimension, i.e. diodes and strip sensors, can be accurately modeled in 2D, and extended to the dimensions of a real device by an appropriate factor. The 3D device structures, although requiring much computing time and processing capacity, are mandatory for reliable simulations of the pixel and 3D-columnar sensors, presented in Figure 5. In a typical parameter scan the number of nodes in the simulation can be 10–20, while the simulation of a single node for a 3D-structure with large enough mesh-size to reproduce a realistic device (e.g. smooth implant shapes at the electrodes) can be in the order of

[4] CMS High Granularity Calorimeter

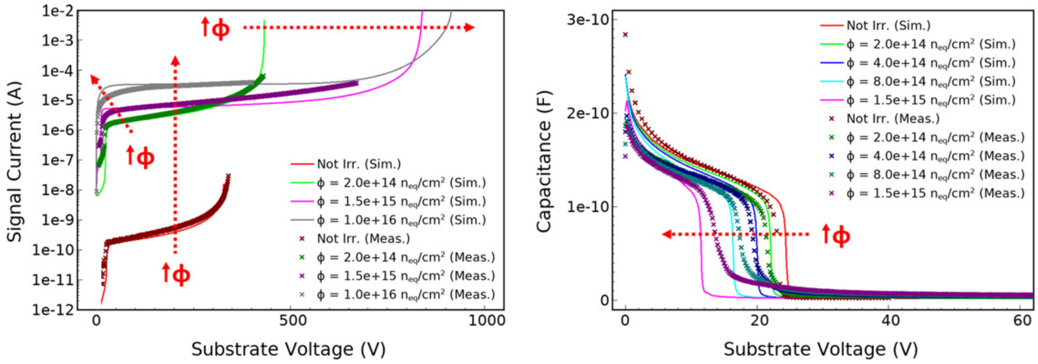
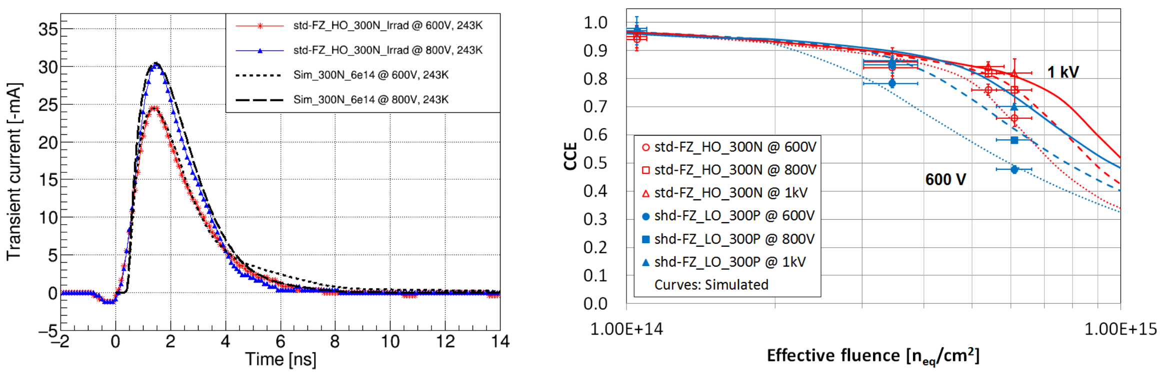


Figure 2. I-V (on the left) and C-V (on the right simulated curves compared with experimental data before and after irradiation for a Low-Gain Avalanche Diode (LGAD) produced by FBK. The sensor area is $1\,\mathrm{mm}^2$, the thickness is $55\,\mu\mathrm{m}$ and the temperature is 300 K. In the simulation, the "New University of Perugia TCAD model" was coupled with an analytic model developed by the Torino group that describes the mechanism of acceptor removal in the multiplication layer.

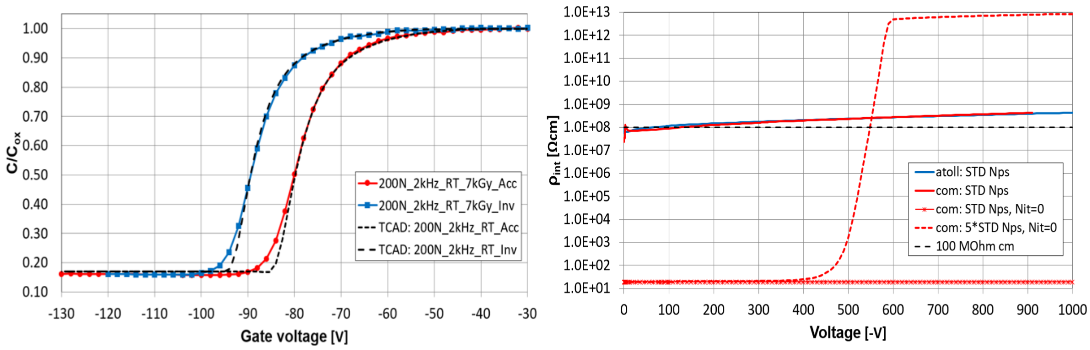


(a) (b)

Figure 3. Examples of bulk-damage modeling [20]. (a) Measured and simulated IR-laser induced transient signals for 300-μm-thick p-on-n pad-sensor (300N) after neutron irradiation to the fluence of $(6.1 \pm 0.5) \times 10^{14}\ \mathrm{n_{eq}cm^{-2}}$. The simulation applied neutron defect model [7] with a fluence of $6.0 \times 10^{14}\ \mathrm{n_{eq}cm^{-2}}$. The sensor parameters used in the simulation were extracted from CV/IV-measurements. (b) Measured and simulated evolution of charge collection efficiency (CCE) with voltage and 1-MeV equivalent neutron fluence for 300-μm thick sensors at -30 °C. Simulated results use dotted, dashed and solid curves for 600 V, 800 V and 1 kV, respectively.

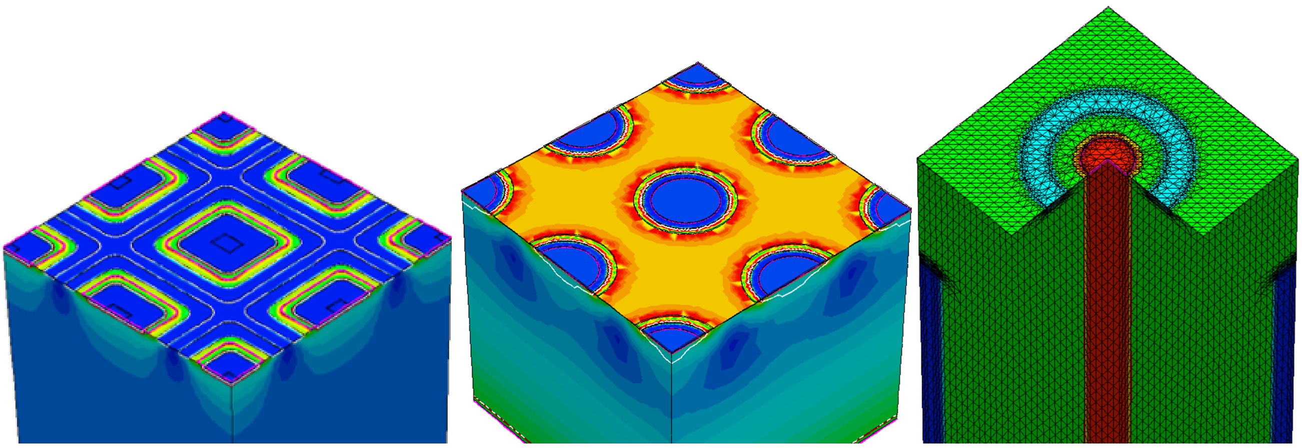
days in a standard multi-core processor. Therefore, considering different options for the optimization of the simulation times is highly motivated.

Speedup investigation of a 3D-device with about 10^6 mesh-points in Figure 6 shows, that shared-memory parallelization benefits simulation execution time by a factor of 5 when the number of threads is increased from 1 to match the number of physical cores in the processor. Further factor of about 3 is gained when the computation method of the physics equations is changed from a direct linear solver (optimal for 2D-simulations) to an iterative linear solver (ILS) with tuned parameters to avoid compromising the accuracy of the simulation results. Weakly supported distributed processing (cluster computing) in



(a) (b)

Figure 4. Examples of surface-damage modeling. (a) Measured and simulated CV-curves of a γ-irradiated 200-μm-thick n-bulk (200N) MOS-capacitor with t_{ox} = 700 nm for the dose of 7.0±0.4 kGy. Measurements included voltages starting from both inversion (Inv.) and accumulation (Acc.) regions. (b) Inter-pad resistivity at -20°C for individual (atoll) and common p-stop isolation implants with HGCAL-parameters, simulated by applying N_{f} and N_{it}-parameters tuned from MOS-capacitor measurements and simulations for the dose of 23.5 kGy. The 100 MΩ·cm (black dashed line) represents conservative estimation for high level of pad isolation. STD N_{ps} = standard value of p-stop peak doping.



(a) (b) (c)

Figure 5. 3D-sensor structures designed in Sentaurus TCAD. (a) Electric fields in a 50 × 50 μm^2 n-on-p pixel sensor for CMS Tracker. (b) Electric fields in a p-on-p MediPix sensor [21] with a 55 μm pitch. (c) Sliced view of a double column-double sided 3D n-on-p sensor with a p-stop isolation. Aluminum and oxide have been stripped from the surface.

Synopsys TCAD is possible to be compensated in a cluster by generating copies of the simulation project that are dedicated for each node of the parameter space and running these simultaneously.

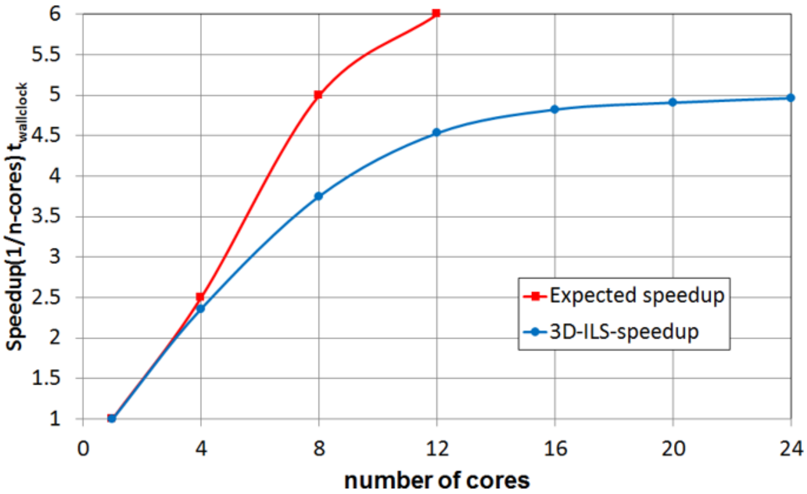


Figure 6. Speedup by shared-memory parallelization in a 3D-detector structure with about 10^6 mesh-points, where the physics equations are solved. Theoretical speedup courtesy of Synopsys support.

3.3 Process Simulations for Device Development(Lipton)

Commercial TCAD packages are capable of full simulations of device fabrication, including epitaxy, implantation, annealing, deposition and oxydation. The accuracy and detail provided by these simulations can be invaluable in the development of new sensor technologies or in understanding the behaviour of existing devices. For devices such as LGADs an accurate model of the implant doping density and profile is crucial to understanding and predicting performance. This is possible with process simulation. The process model can also provide a link between commercial foundries and instrumentation developers.

3.4 Testbeam

Sensor simulations from commercial packages like `TCAD` are less often used for Monte Carlo simulations of drift and diffusion of carriers or, for example, simulations of beam tests at facilities with charged particle beams. For such purposes, specialized Monte Carlo software is used. These Monte Carlo simulation packages can use sensor simulations results such as the sensor electric field as input; see for example [22].

One example of a software package for drift and diffusion modeling of carriers in silicon sensors is `Pixelav` [4, 23, 24], originally created for interpretation of data taken with both unirradiated and irradiated sensors at pion test beams. This package has accurate models of charge deposition and transportation and can simulate charge drift under magnetic fields. It also models radiation damage with the trapping of charges. It uses input electric fields from the `TCAD` simulation software. `Pixelav` is now used as standalone software in the CMS template-based hit reconstruction software that includes radiation damage simulation [25–28]. In the templates created with `Pixelav` provide both corrections to the hit position and the cluster charge.

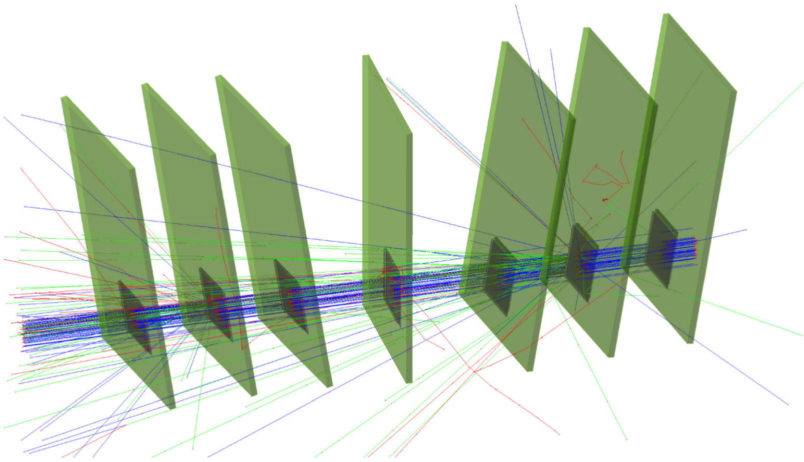


Figure 7. Visualization of a simulated detector telescope setup with 7 planes. in `Allpix`^{2}. The beam is incident from the right, and the colored lines are the primary and secondary particles propagated through the setup by the simulation. Figure from [31].

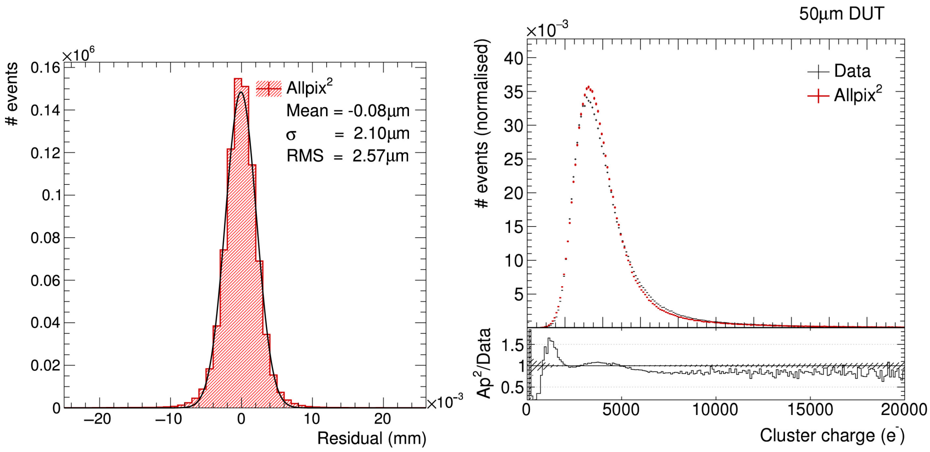


Figure 8. Residuals and cluster charge distribution simulated with the `Allpix`^{2} software package compared to data. The cluster charge is for a 50 μm device under test (DUT). The residuals are the difference between the reconstructed telescope track position in the DUT and the true hit position of the simulated particle. Figures from [31].

Packages similar to `Pixelav` are `Allpix` [29] and `KDetSim` [30]. `KDetSim` is based on the CERN `ROOT` software package. It is fast, allows for simulation of larger volumes, and allows for iterative approaches. All packages are free and open source.

Another free and open source package that includes experimental setups such as beam telescopes and their material effects like multiple scattering and nuclear interactions based on `Geant4` is `Allpix`^{2} [31]. This includes energy deposition based on `Geant4`, drift and diffusion for charge propagation, and models charge digitization. A visualization of a setup provided by the software package is shown in Fig. 7. The `Allpix`^{2} framework can also provide observables for comparison with test beam data such as particle clusters, tracks, residuals, and cluster charge. An example is shown in Fig. 8. The packages now also includes different charge carrier mobility models and the possiblity to load doping profiles for doping-dependent charge carrier lifetime calculations [32], and foresees to include trapping of charges.

3.5 Full detector systems

ATLAS approach (modified digitization), CMS approach (efficiency corrections), LHCb approach (tuned charged transport)

Within large HEP collaborations, such as those of the Large Hadron Collider experiments, silicon detector simulation is typically performed using proprietary software written within the experiment's software framework (for example Athena, Gaudi, and CMSSW for ATLAS, LHCb and CMS respectively). Even within a single framework, multiple different approaches may exist which have been tailored for a specific use-cases.

Detailed detector performance studies typically need the most detailed approach available, which comes at the cost of significant highly processing times. Such studies can generally be performed to a sufficient level of precision by using smaller samples sizes and/or a limited set of physics processes. This is not the case for the production of Monte Carlo samples for use in data analyses, where large samples covering a wide range of signal and background processes are needed.

Using fully-detailed approaches for production of physics analysis Monte Carlo samples can therefore sometimes become prohibitive, and this will increasingly become the case for High-Luminosity LHC. Faster and more approximate approaches therefore also need to be made available to be used in the production of such samples, potentially with different approaches being used for signal processes to those used for backgrounds, or the minimum bias collision events used to represent the large number of additional 'pile-up' interaction per bunch crossing which accompany the signal process. In certain circumstances, different levels of detail may be considered at different positions within the detector, with a more accurate modeling applied for crucial measurements close to the particle interaction point, or in areas of high particle flux.

The faster, more approximate methods will typically rely on a parameterization or templates derived from the fully-detailed approach, stand-alone simulations, or from data. Appropriate and robust procedures for making comparisons of key observables between the different approaches and also crucially between experiment-specific and stand-alone software are therefore highly beneficial for this process.

One aspect of silicon detector simulation which is becoming increasingly important is the modeling of radiation damage. A number of different approaches to this topic have been taken:

- A *modified digitization* approach has been employed by ATLAS, in which specific adaptations are made within the code responsible for modeling charge generation and transport within the sensor, in order to account for the effects of radiation damage on the generated charges prior to their readout.

- CMS takes a different approach, in which *cluster templates* are derived based on comparing the properties of charge clusters produced in independent simulations with and without radiation damage effects. These templates are parameterized according to pertinent factors such as particle incident angle, and position within the detector, in order that appropriate efficiency corrections can be applied to channels within the clusters produced without explicit radiation damage modeling applied.
- LHCb uses *tuned charged transport*

4 Challenges and Needs

- Unified radiation damage (TCAD) and annealing model
- Prescription for uncertainties in TCAD models
- Measurements of damage factors (many of the inputs in the RD50 database are based on simulation or less)
- Update to basic silicon properties? https://cds.cern.ch/record/2629889
- How to deal with proprietary software and device properties? The `Weightfield2` [33] package provides and alternative to TCAD. Its limitations are ...
- Feedback between full detector systems and per-sensor models
- Extreme fluences of future colliders
- Balancing modeling accuracy against processing time overheads (different approaches likely needed for different applications even within the same experiment)

Acknowledgments

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