Statistical Enhancement (Variance Reduction) for Monte Carlo Simulation

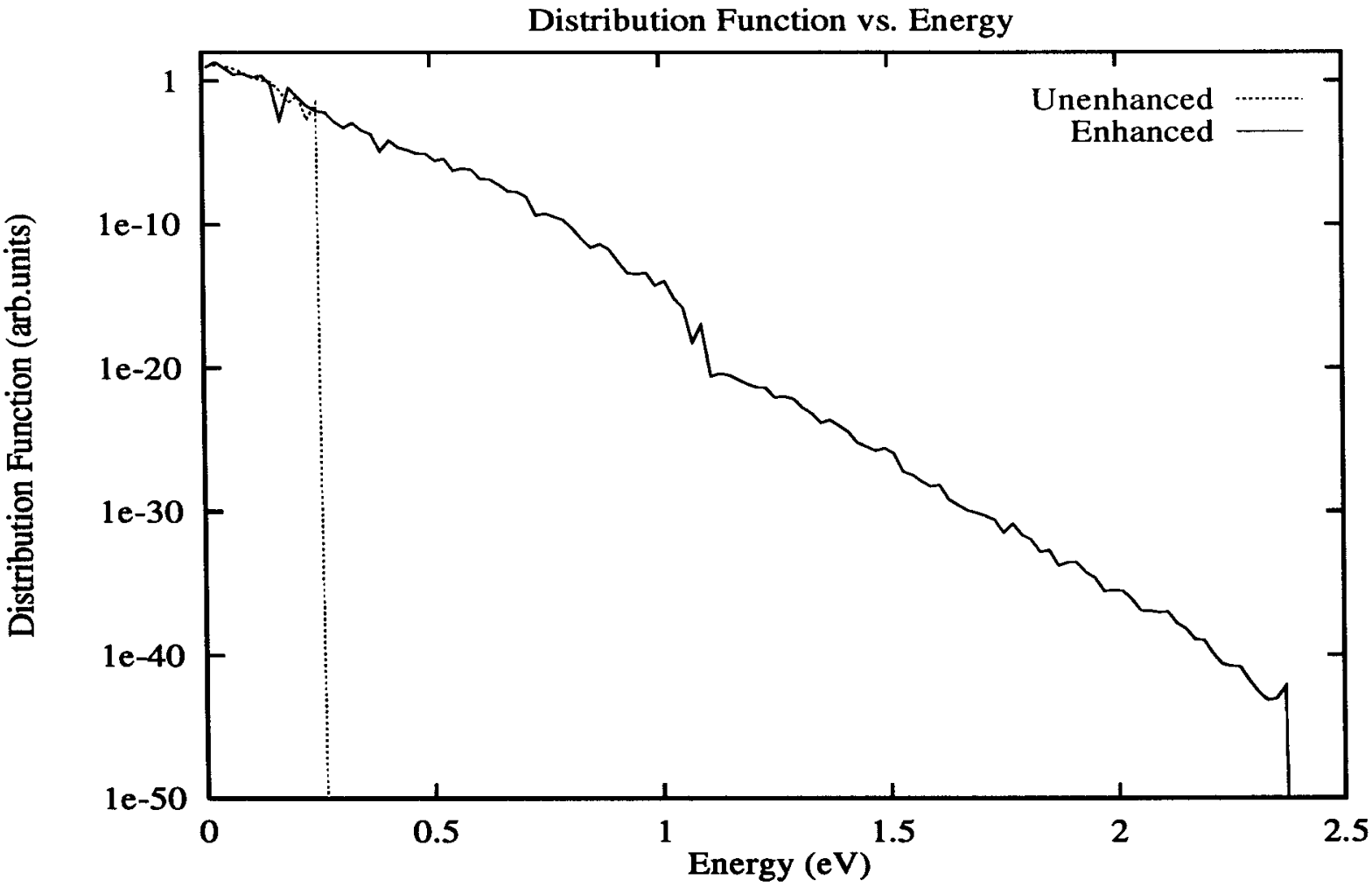
Umberto Ravaioli

Beckman Institute and
Department of Electrical and Computer Engineering
University of Illinois at Urbana-Champaign
Urbana, IL 61801, USA

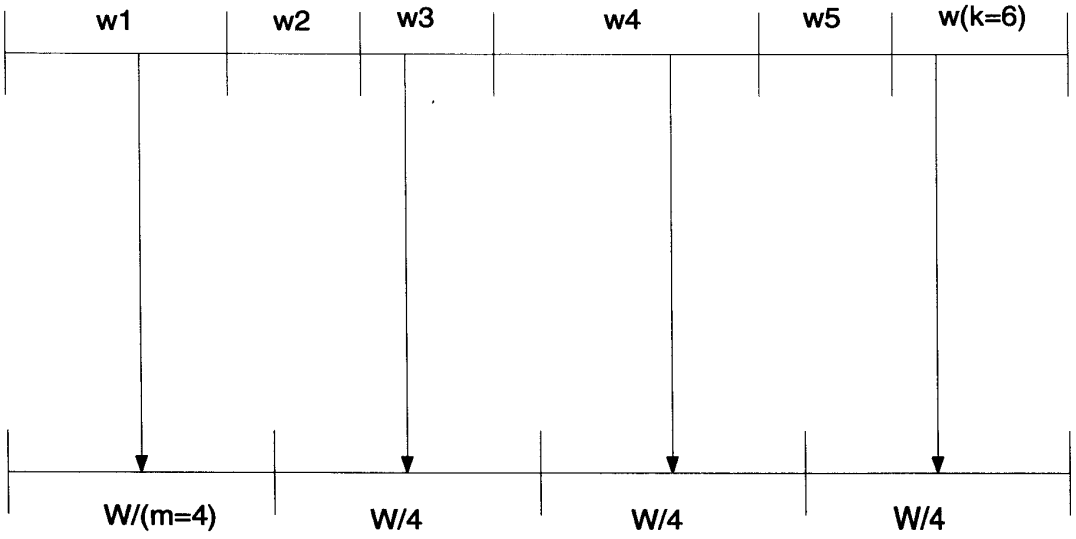
Monte Carlo simulation is noisy

- **Some of the noise is “real” and reflects the true nature of the conduction processes**
- **Some noise may be “numerical”, due to the difficulty in having a large enough sample to collect needed statistics.**
- **Statistical enhancement is applied to remove particles where they are “oversampled” (real space or momentum space) and add particles where they are ”undersampled”; or different weights are assigned to particles, so that rarely populated regions may have many particles with small weight, and highly populated regions may have few particle with large weight.**
- **Typical application is the resolution of high energy tails ofthe carrier distribution.**

Effects of Statistical Enhancement

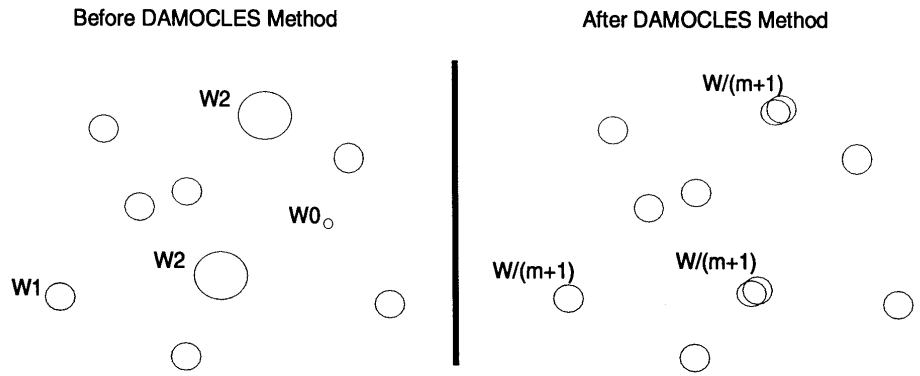


Multi-Comb Method



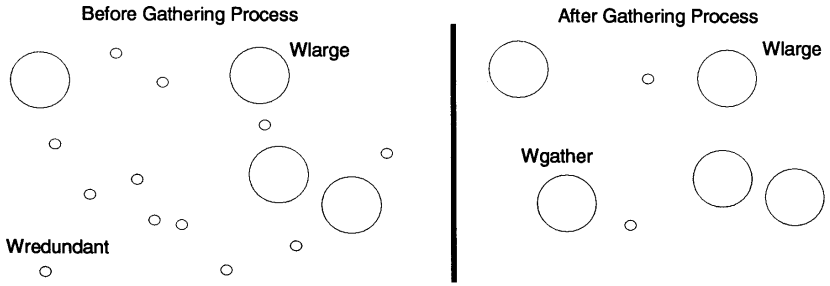
- $k(=6)$ variable-weight particles are combed into $m(=4)$ identical-weight particles with weight $W/m(=4)$, where $W = \sum_{i=1}^{k(=6)} w_i$.
- The target number of particles per bin, m, is chosen in this study as the total number of particles divided by the number of occupied bins.
- All allocated particle memory is used throughout the simulation.
- Following a Multi-Comb, all particles in a phase-space bin have the same weight, W/m.

DAMOCLES Method



- If a bin is unoccupied, the weight of the bin, w_b, is set to zero.
- If a bin is occupied but w_b is zero, w_b is set to the average weight of particles in the bin.
- If $w_i < w_b$, the w_i-weight particle is retained with probability $\frac{w_i}{w_b}$ as a w_b-weight particle and is removed with probability $1 - \frac{w_i}{w_b}$.
- If $w_i > w_b$, the w_i-weight particle is replaced with $\zeta = int(\frac{w_i}{w_b})$ w_b-weight particles with probability $1 + \zeta - \frac{w_i}{w_b}$, or $\zeta + 1$ w_b-weight particles with probability $\frac{w_i}{w_b} - \zeta$.
- The target number of particles per bin, m, is again chosen as the total number of particles divided by the number of occupied bins.
- If the number of particles in a bin falls outside $\pm 20\%$ of the target number, particles are split or rouletted to change to approximately the target number.
- Following a DAMOCLES enhancement, all particles in a phase-space bin have the same weight.

Adaptive Gather Method



- Particles (over all bins) are identified as "redundant" if they are smaller in weight than a larger particle in the same bin by the ratio *relthre* (=0.05 in this study).
- Using the set of redundant particles, groups of up to n (=10 in this study) may be gathered (grouped together as a single particle) if their weights differ by no more than *ratio* (=2 in this study).
- The target number of particles per bin is determined by the method (rather than chosen by the user) as 80% of the total number of particles over the number of occupied bins.
- In bins with occupation lower than target number, particles are split to match the target number.
- 80% of all particles are evenly distributed across all occupied bins and 20% of all particles are left in bins of the largest population.
- The gathering process allows the method to use all allocated particle memory throughout the simulation.
- Following an Adaptive Gather, all particles in a phase-space bin do not necessarily have the same weight.

Test Runs for comparison of the techniques

Bulk simulation for undoped silicon, with 30,000 particles

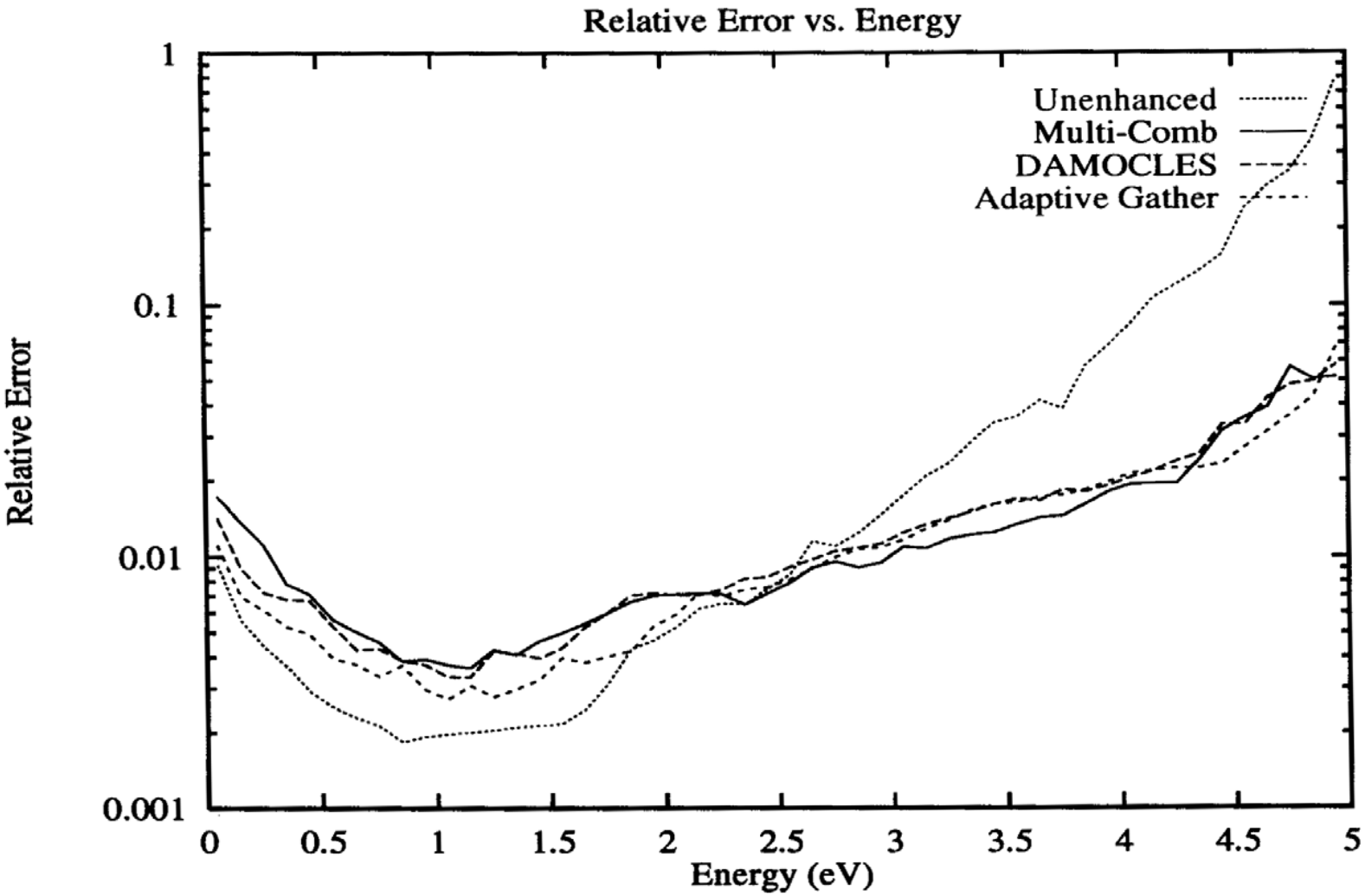
Electric field 300 kV/cm

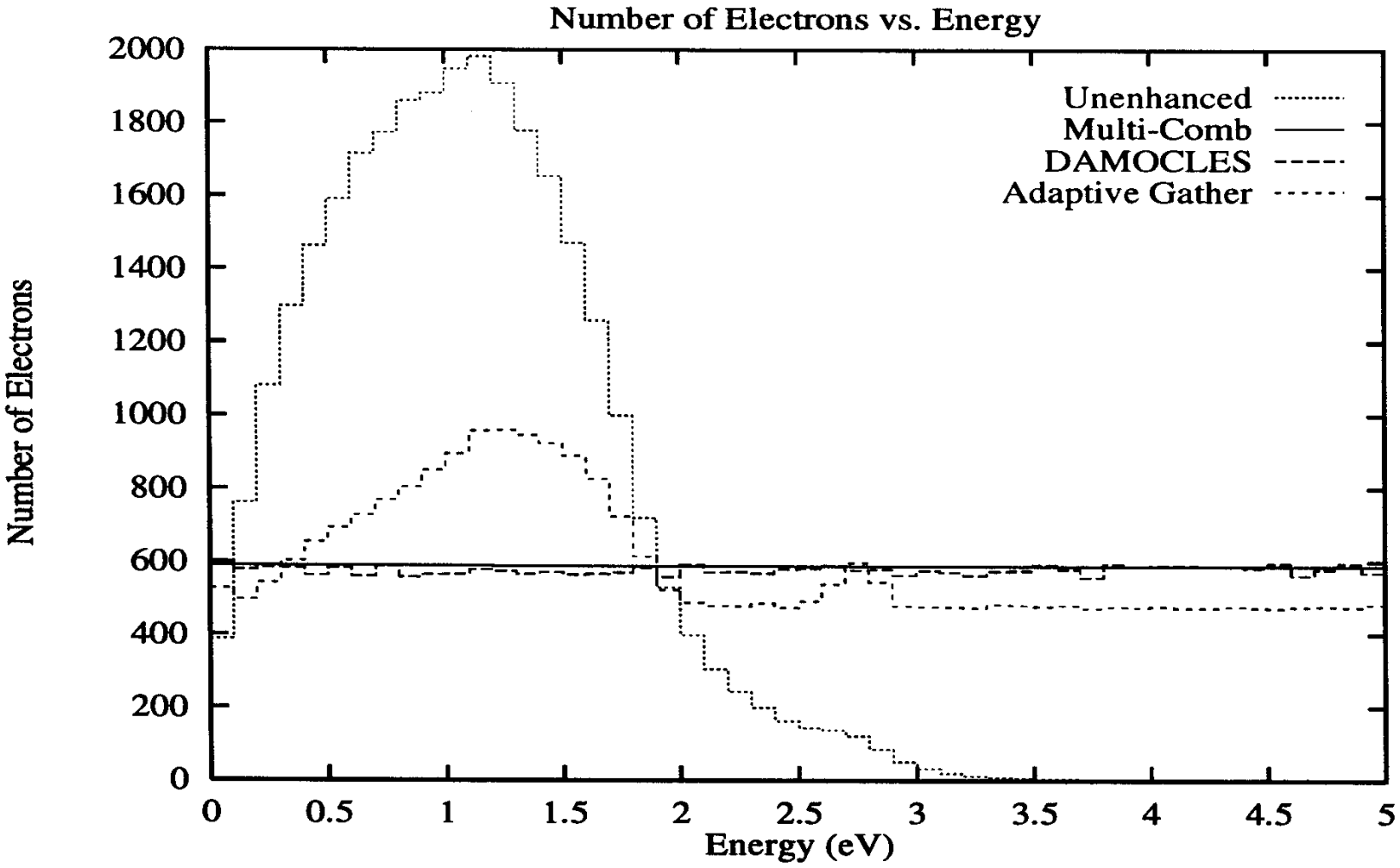
50 energy bins of width 0.1 eV from 0 to 5 eV

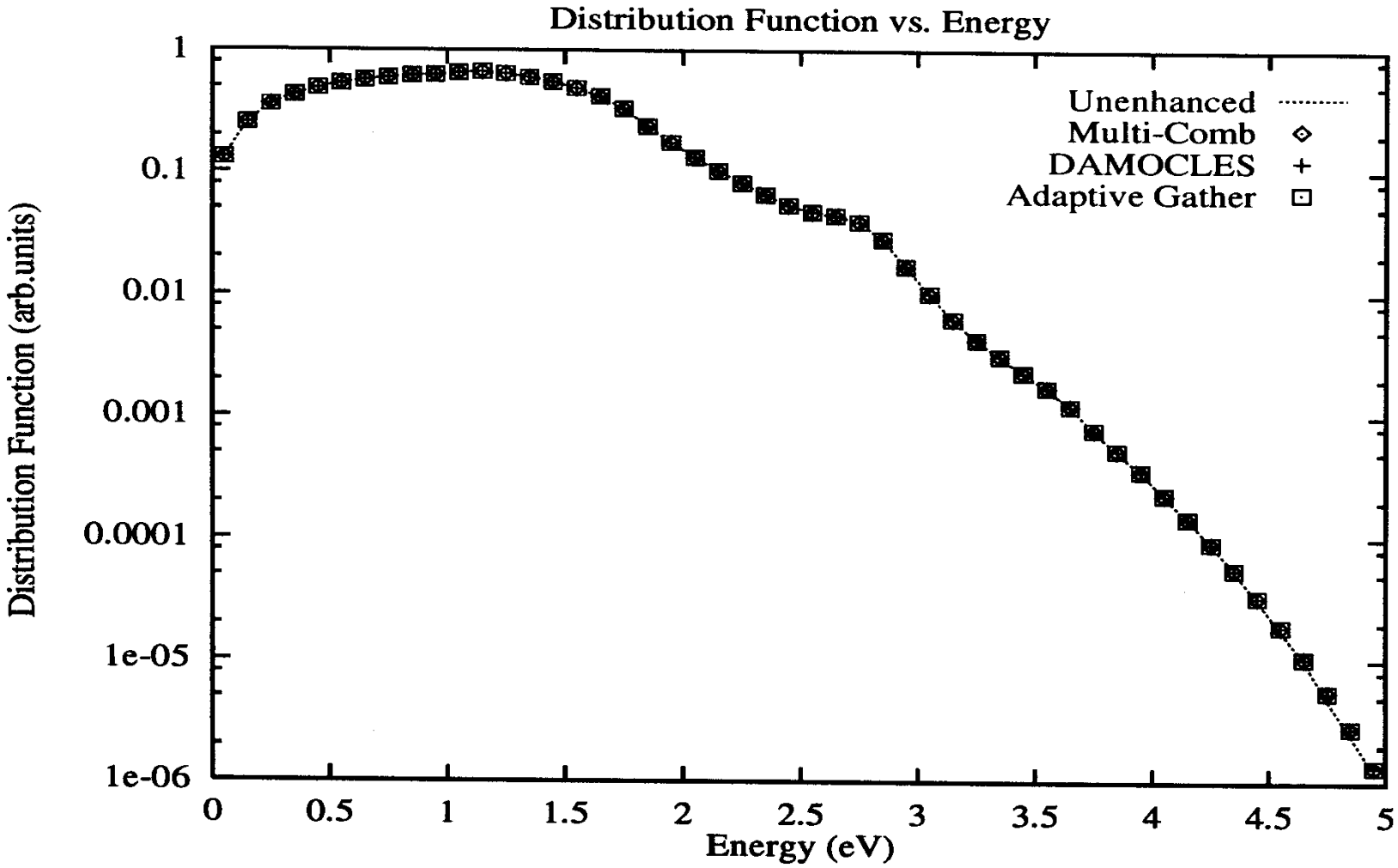
Enhancement called every 1fs of simulation

Results were averages of 50 independent simulations of 3000 fs

Error performance analysis was done for steady-state, ignoring the initial 500 fs of the simulation.


Relative Error vs. Energy
Unenhanced
Multi-Comb
DAMOCLES
Adaptive Gather
Relative Error
1
0.1
0.01
0.001
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
Energy (eV)


Number of Electrons vs. Energy
Number of Electrons
Energy (eV)
Unenhanced
Multi-Comb
DAMOCLES
Adaptive Gather
0
200
400
600
800
1000
1200
1400
1600
1800
2000
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5


Distribution Function vs. Energy
Distribution Function (arb.units)
Energy (eV)
Unenhanced
Multi-Comb
DAMOCLES
Adaptive Gather
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5