SAND2011-7122C

Stochastic Richardson Extrapolation as applied to Vlasov-Poisson Child-Langmuir Diode Verification Example

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Purpose/Goals

- Develop a validation methodology that applies to stochastic multi-physics plasma problems

- Brief overview of target application
- Vlasov-Poisson Child-Langmuir diode
  - Apply this methodology to a verification problem

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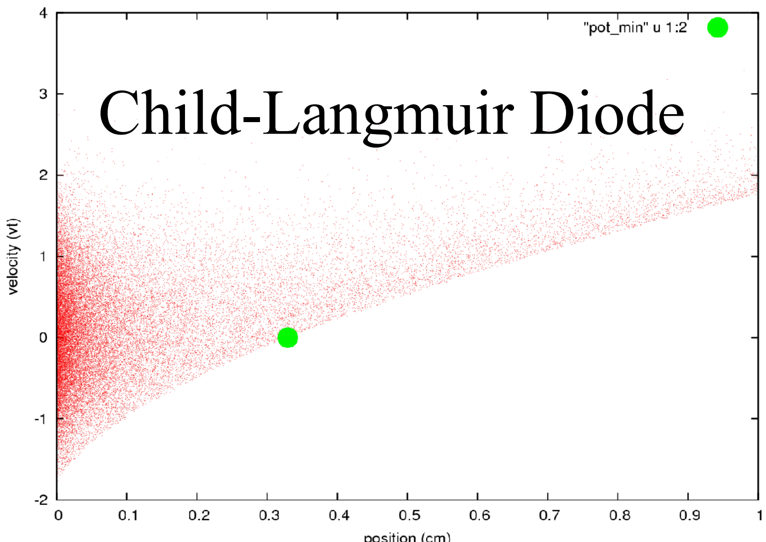
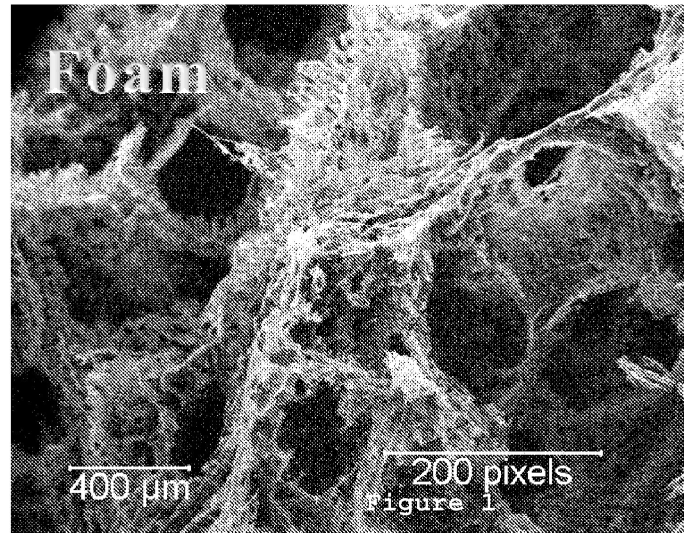
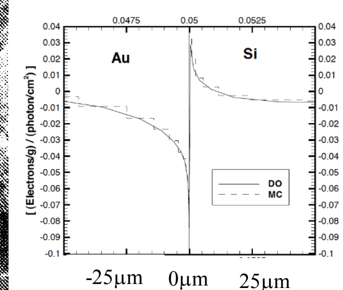
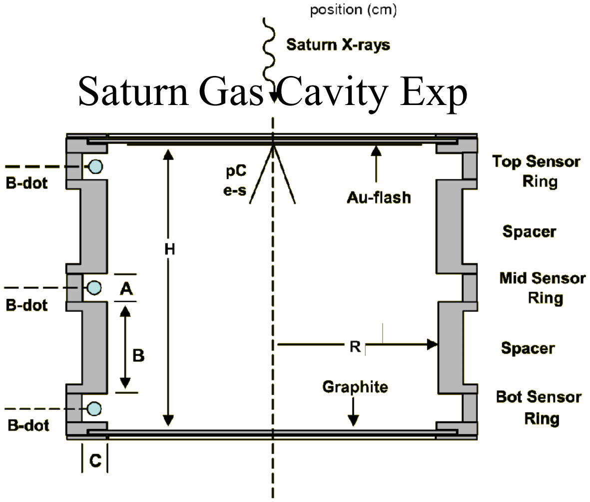
Stochastic Applications Under Investigation



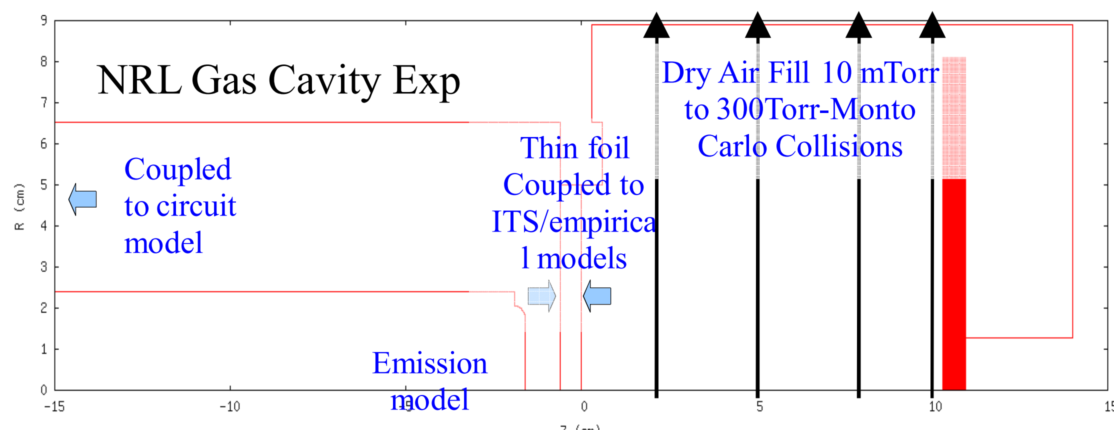




Charge deposition at material boundaries



A = 1.6 cm, B = 5.08cm, C = 1.415 cm, H = 15.63 cm, R = 9.005 cm



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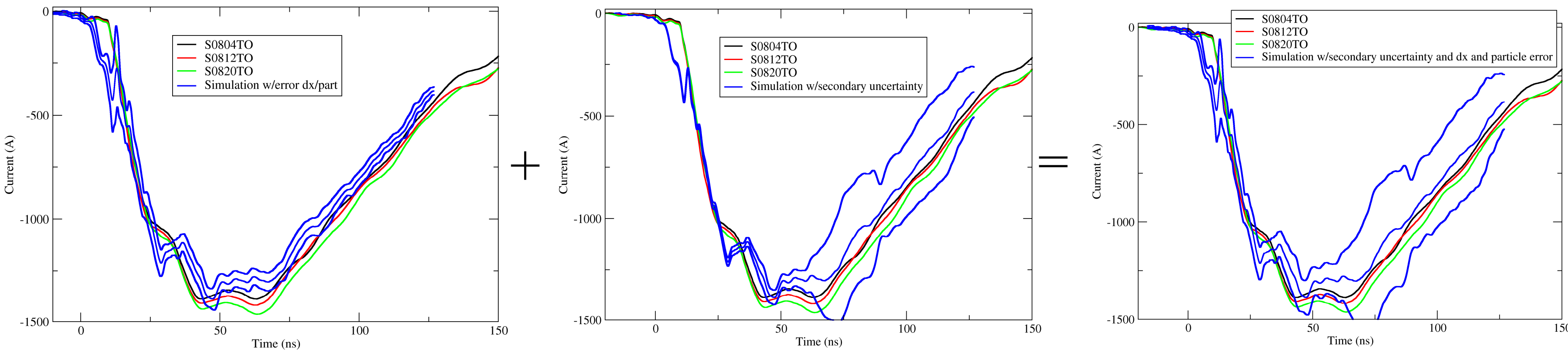
Numerical Uncertainty: Only One Part of the Problem

- Epistemic Loop (includes model form)
  - Aleatory Loop
    - Numerical Error Estimation Loop
      - Simulation Code

DAKOTA (Epistemic Loop and Aleatory Loop)



Assume the epistemic/aleatory and numerical error loops are independent

24 simulations | 2400+ simulations, Coarse resolution | 2424 simulations

Exo-scale Thoughts

If epistemic/aleatory loops are not independent of numerical error the total number cores used could be 2 billion (7.5M runs x 256 core simulations)

or

44,579 redskys

or

22.5 EFLOPs

Versus independent epistemic/aleatory loops and numerical error

1.5 PFLOPs

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Outline of These Slides

- Diode problem setup
- Least Squares Fit Extension of Richardson Extrapolation
  - Weighting different values
  - Higher order terms
- Stochastic extension of Richardson Extrapolation
  - Determination of error bounds (weighting) on parameters estimated from a distribution
  - Using multiple values

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Vlasov-Poisson Child-Langmuir Diode

- Thermal emission from the left hand side

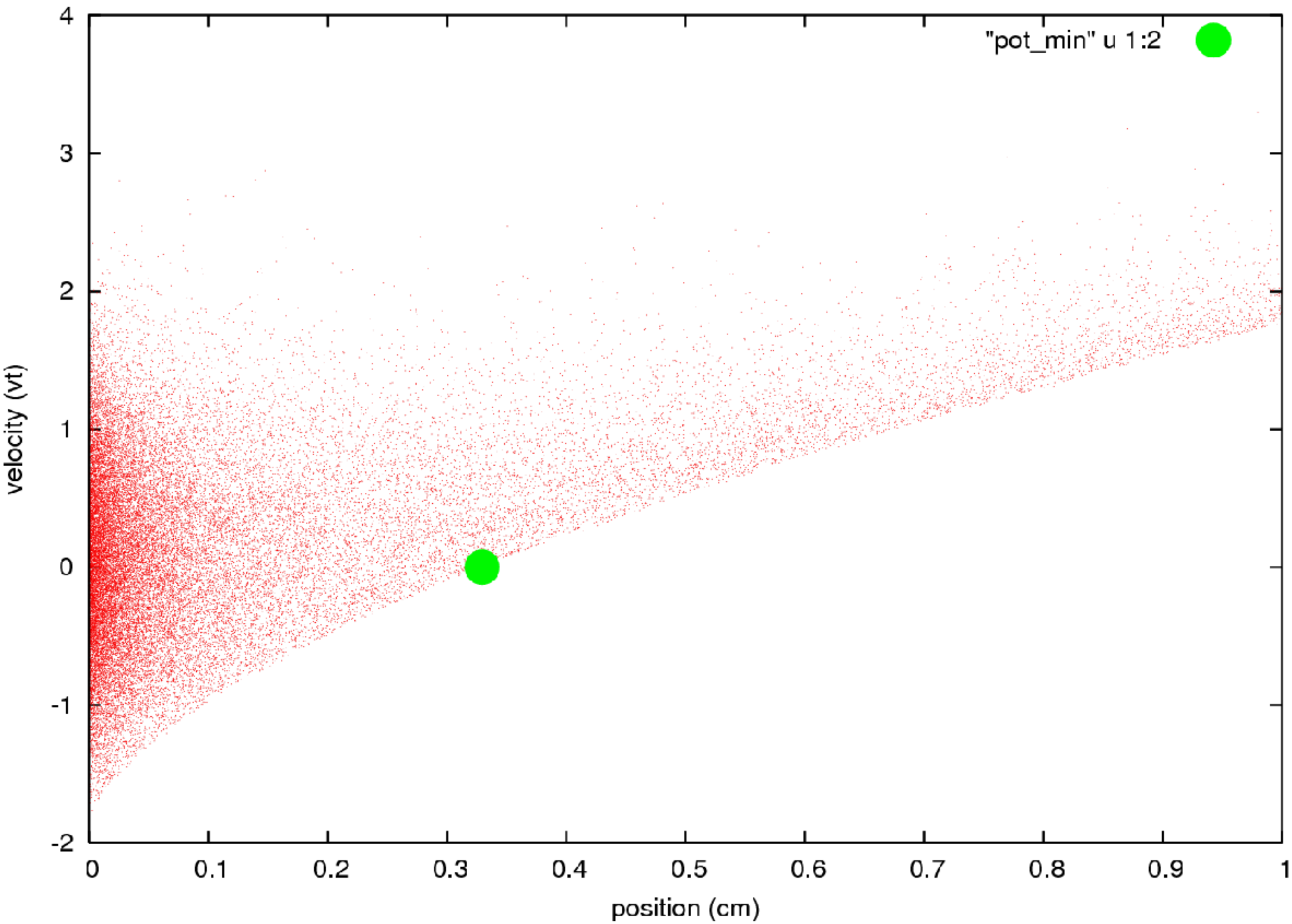
$$f(x=0,v)=\frac{2n_0}{v_t\sqrt{\pi}}e^{-v^2/v_t^2}$$

- Both sides grounded $\phi(0)=\phi(L)=0$
- Injected current, ramped over 20 ns $I=\frac{aq_e n_0 v_t}{\sqrt{\pi}}$
- Pick some dimensions for the simulation
  - L=.01m, A=.02m^2
  - I=10 Amps, v_t=1.876x10^6 m/s (10eV)
- Setup to have about 4% of the current transmitted through the ‘sheath’

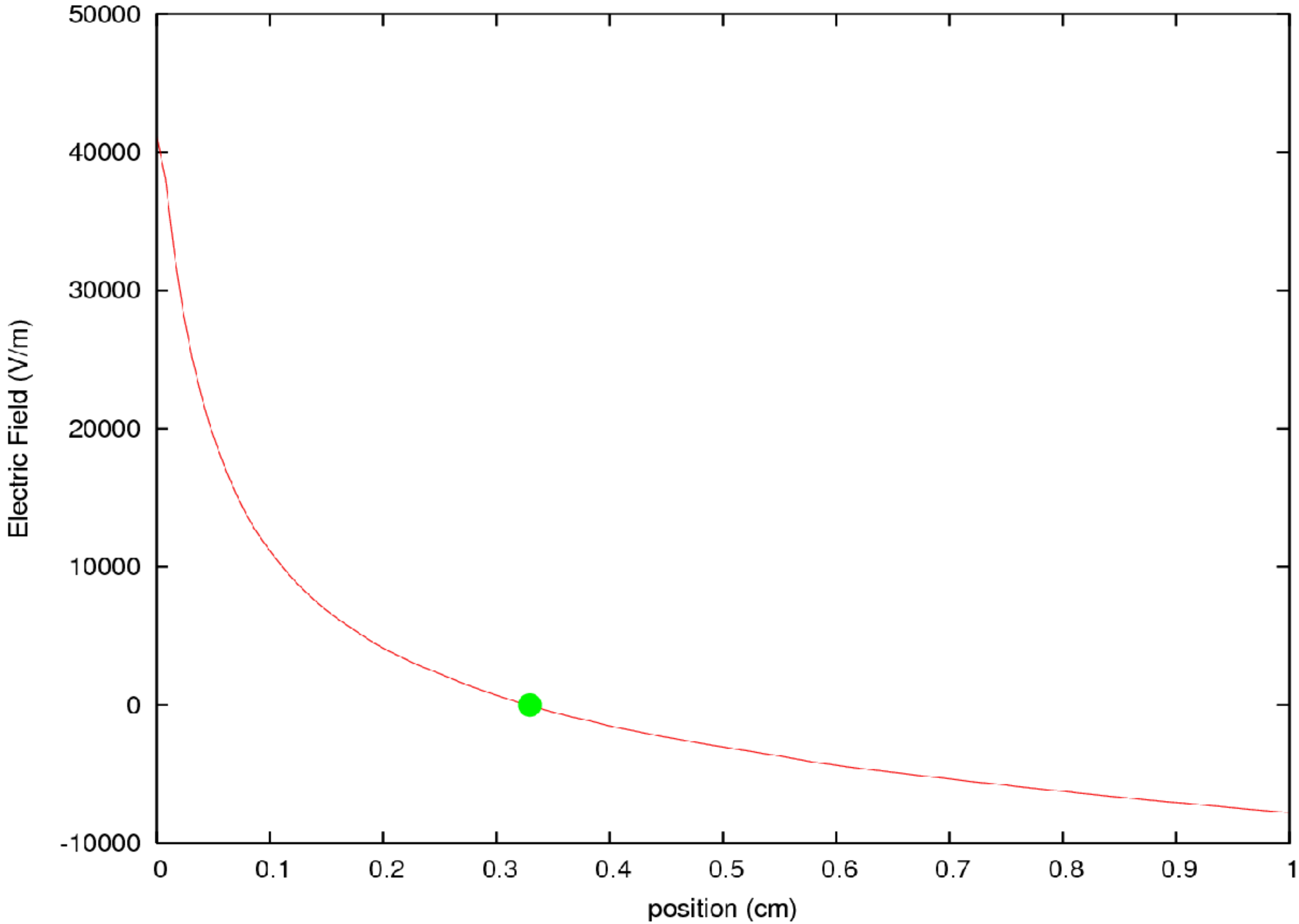
System Response Quantities

- ◆Current transmitted (0.438584 Amps)
- Shot noise of the current (0.0000126577)
- Potential minimum position (0.329428 cm)
- Distribution function at the cathode and anode

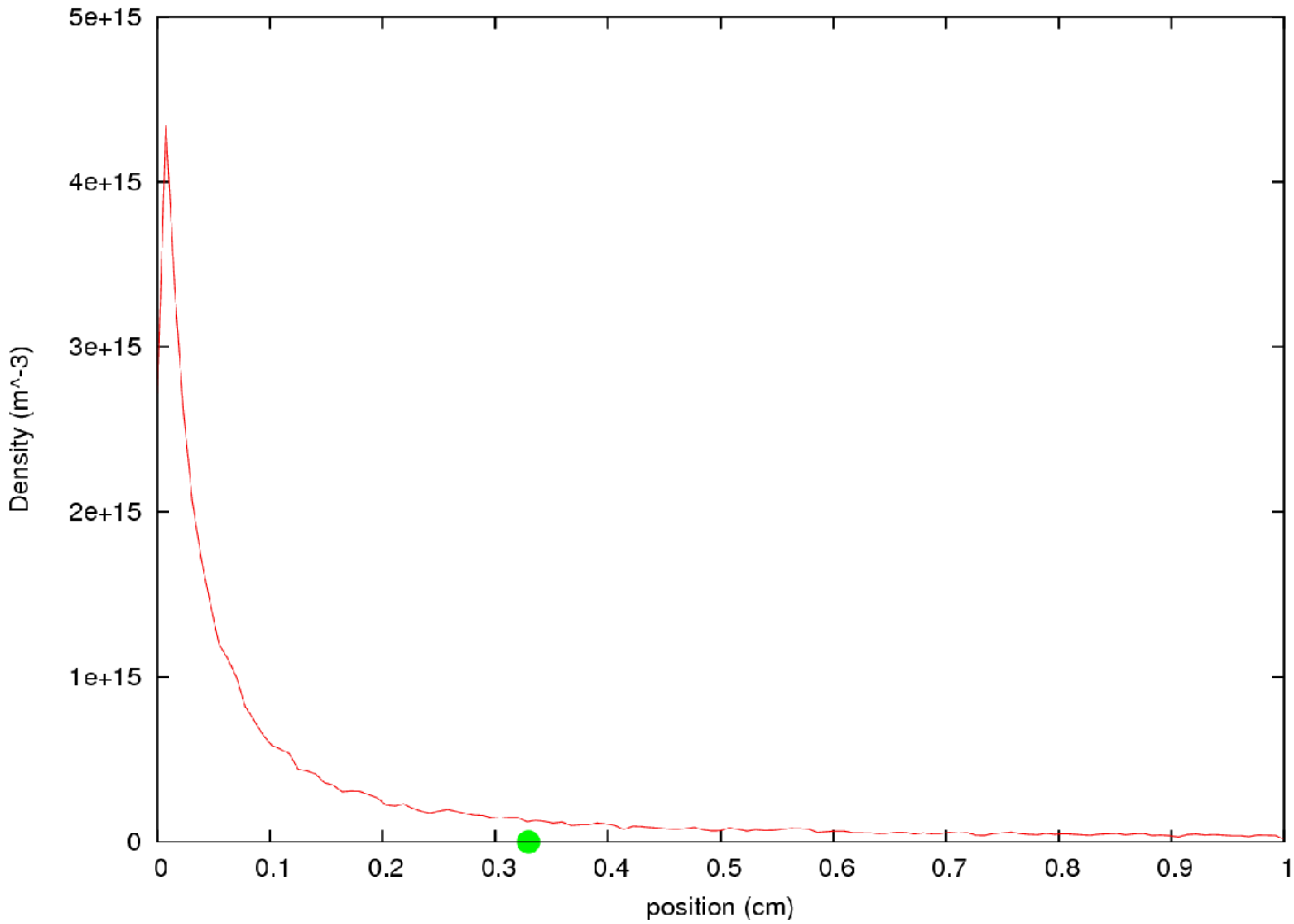
Overview of the Results



Electric Field



Density


5e+15
4e+15
3e+15
2e+15
1e+15
0
Density (m^-3)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
position (cm)

Richardson Extrapolation

General two parameter expansion:

$$
\begin{aligned}
I_{sim} - I_{exact} = & \left(\alpha_0 + \alpha_1 \Delta x^{n_s} + \alpha_2 \Delta x^{n_s+n} + \alpha_3 \Delta x^{n_s+2n} + \cdots\right) \\
& + MPW^{m_s} \left(\beta_0 + \beta_1 \Delta x^{n_s} + \beta_2 \Delta x^{n_s+n} + \beta_3 \Delta x^{n_s+2n} + \cdots\right) \\
& + MPW^{m_s+m} \left(\gamma_0 + \gamma_1 \Delta x^{n_s} + \gamma_2 \Delta x^{n_s+n} + \gamma_3 \Delta x^{n_s+2n} + \cdots\right) \\
& + MPW^{m_s+2m} \left(\delta_0 + \delta_1 \Delta x^{n_s} + \delta_2 \Delta x^{n_s+n} + \delta_3 \Delta x^{n_s+2n} + \cdots\right) \\
& \vdots
\end{aligned}
$$

m_s=starting power for particles, series in m
n_s=starting power for cells, series in n
MPW: macro particle weight
Δx: mesh size

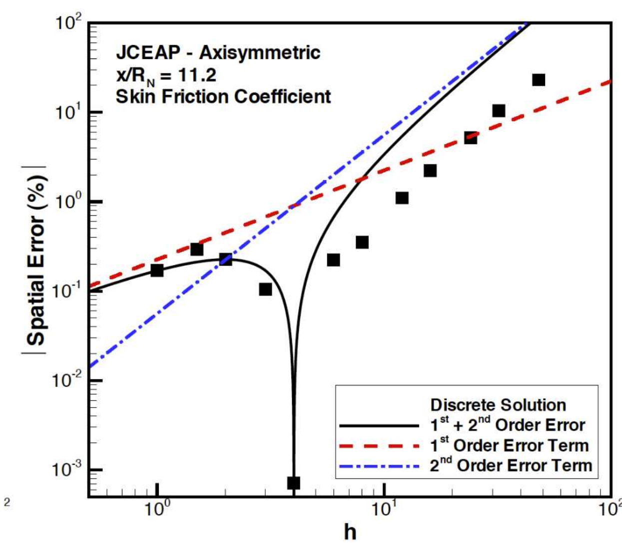
Richardson Extrapolation

Minimum needed for Richardson Extrapolation:

$$I_{sim} - I_{exact} = \alpha_1 \Delta x^{n_s} + \beta_0 MPW^{m_s} + \beta_1 \Delta x^{n_s} MPW^{m_s}$$

Have not seen an improvement in the fit by keeping more terms

- Not fine enough sampling in Δx and MPW
- Higher order RE is fitting “noise”



Review of Discretization Error Estimators in Scientific Computing, Chris Roy, AIAA January 2010

Parameter Uncertainty Estimation

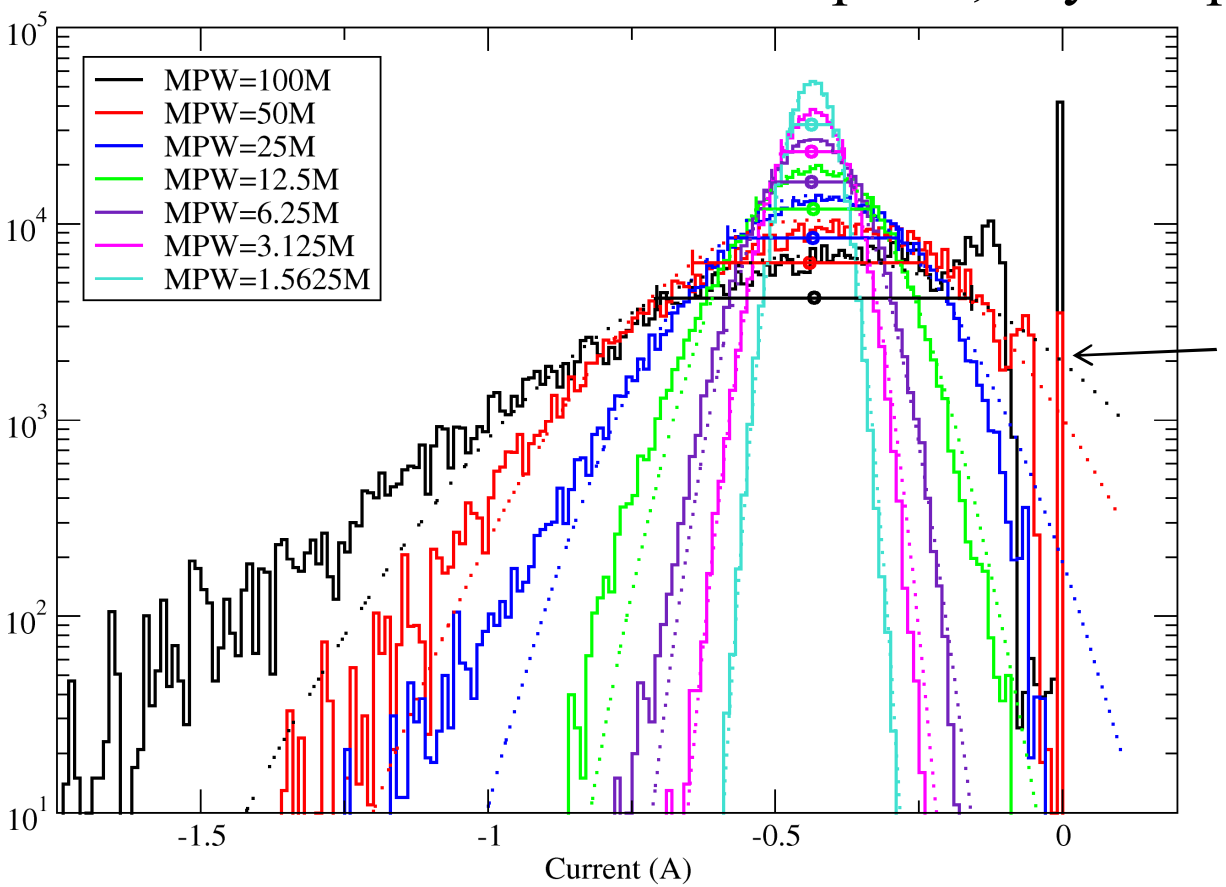
Divide the parameter estimation uncertainty/error into two parts

- **Uncertainty due to finite number of particles sampling the distribution function**
  - **Simulation Measurement Uncertainty**
- **Error in the distribution function due to finite number of particles, finite cell size, and finite time step**

Distribution of Current

64 cells across the diode

Current measurement at mid-plane, beyond potential minimum

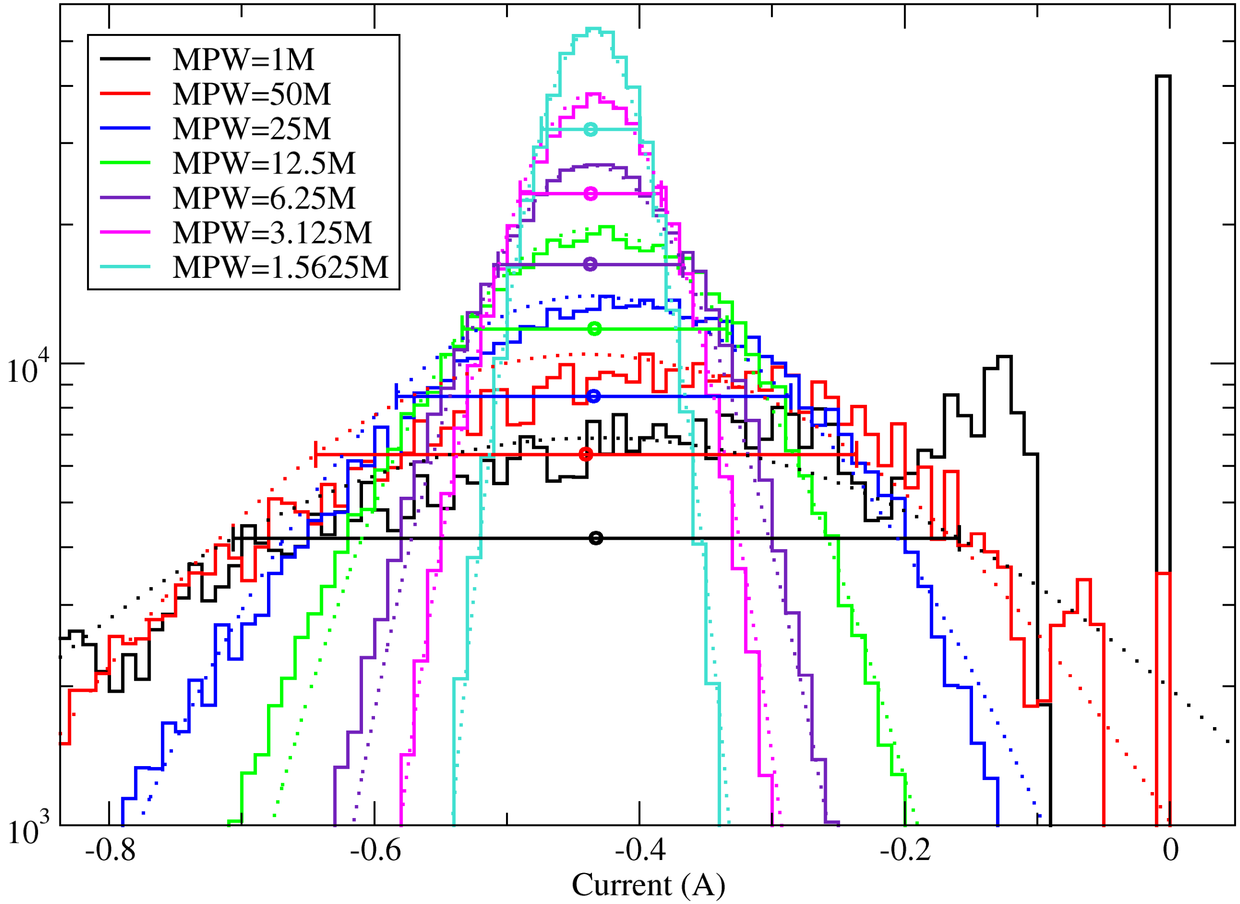


Because the measurement plane is beyond the potential minimum the current can only have a zero or negative value

Could redo these runs with the measurement at ¼ of the way across the diode before the potential minimum

Close-up of Peak

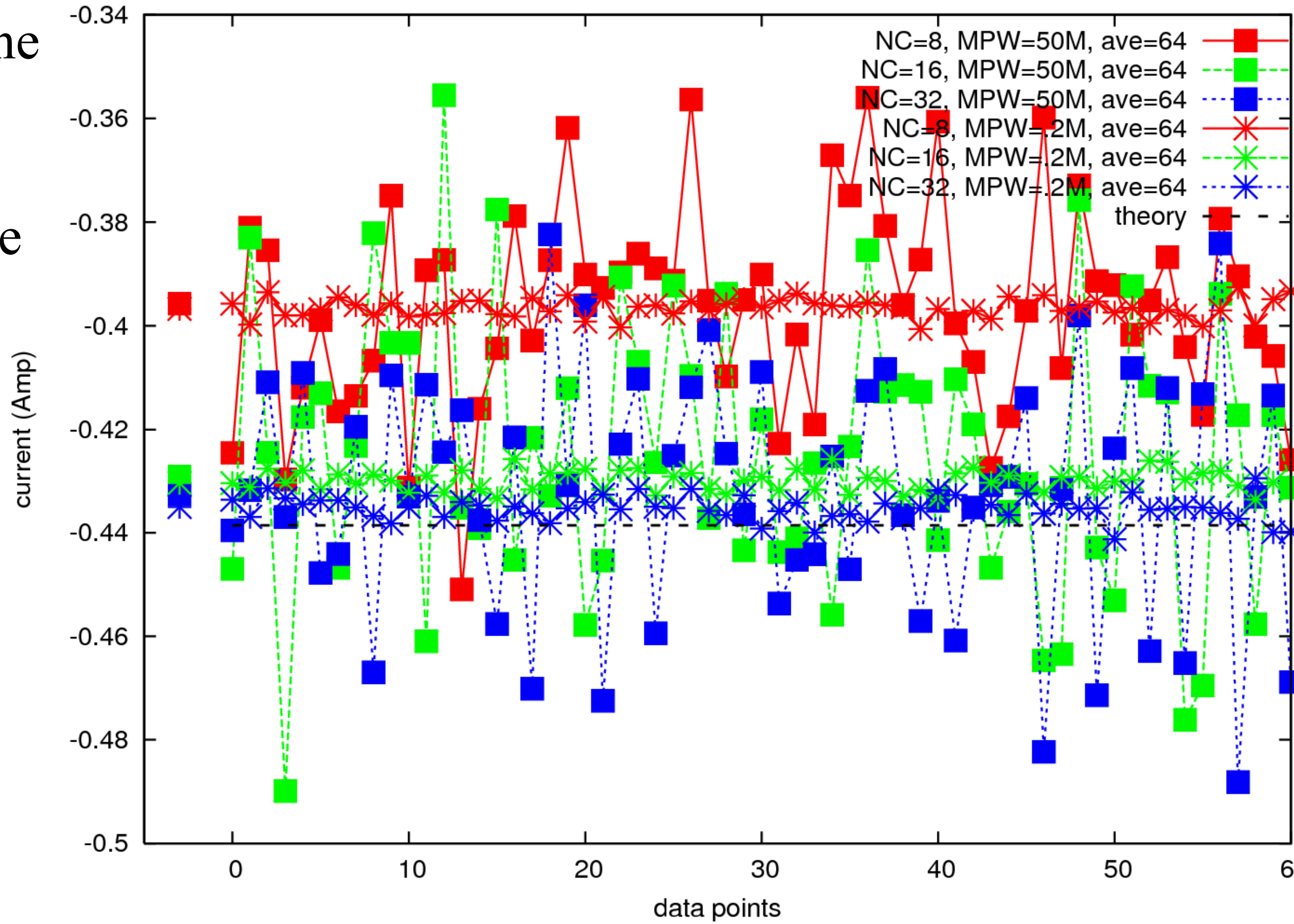
There are systematic differences between the current distribution in the simulation and the Gaussian's show in dots



Moments of the distribution can also be used to compare to Gaussian or to show convergence but doesn't show the shape of the distribution

Number of Particles and Average Convergence

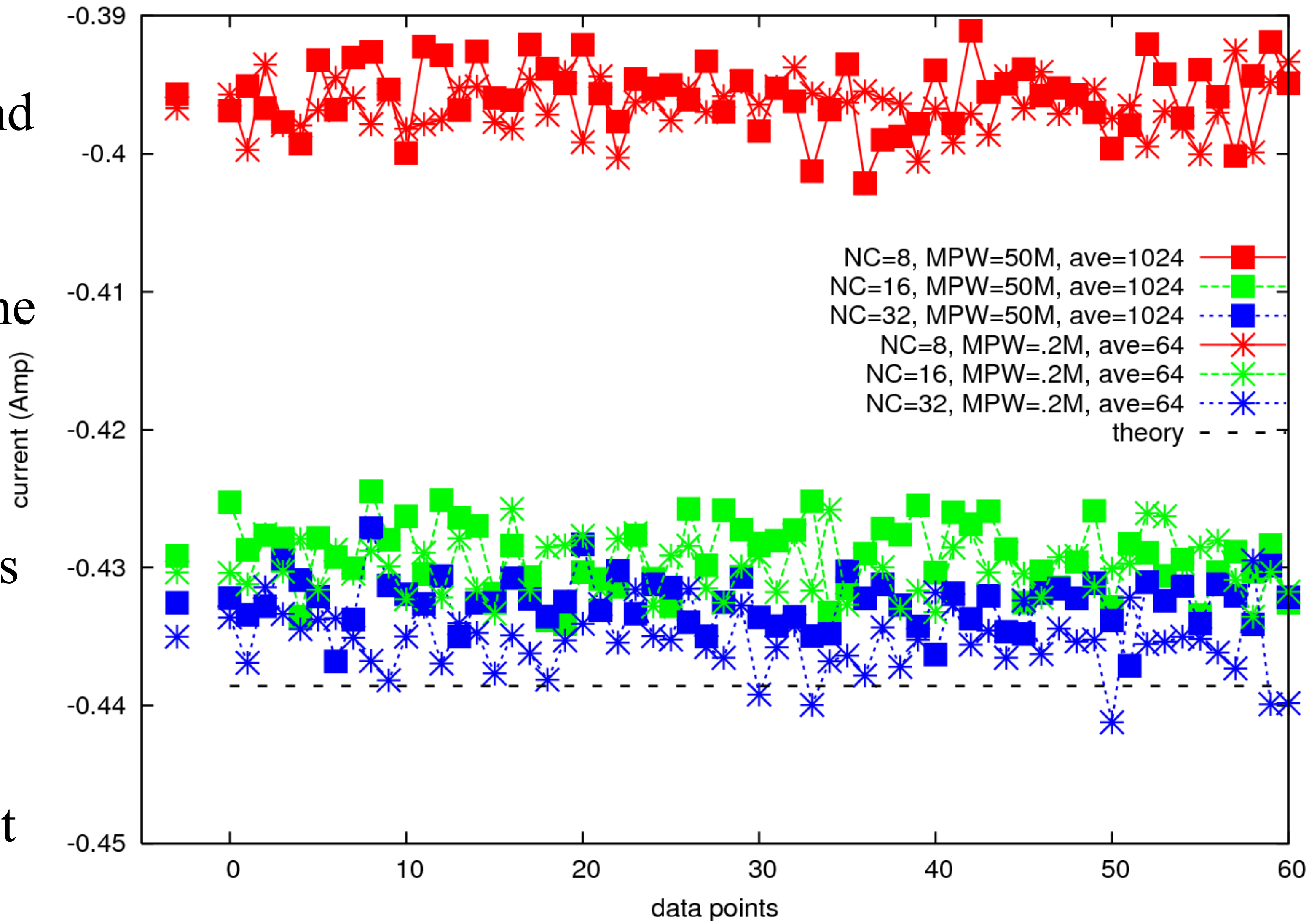
Increasing the number of particles decreases the noise



Number of Particles and Average Convergence

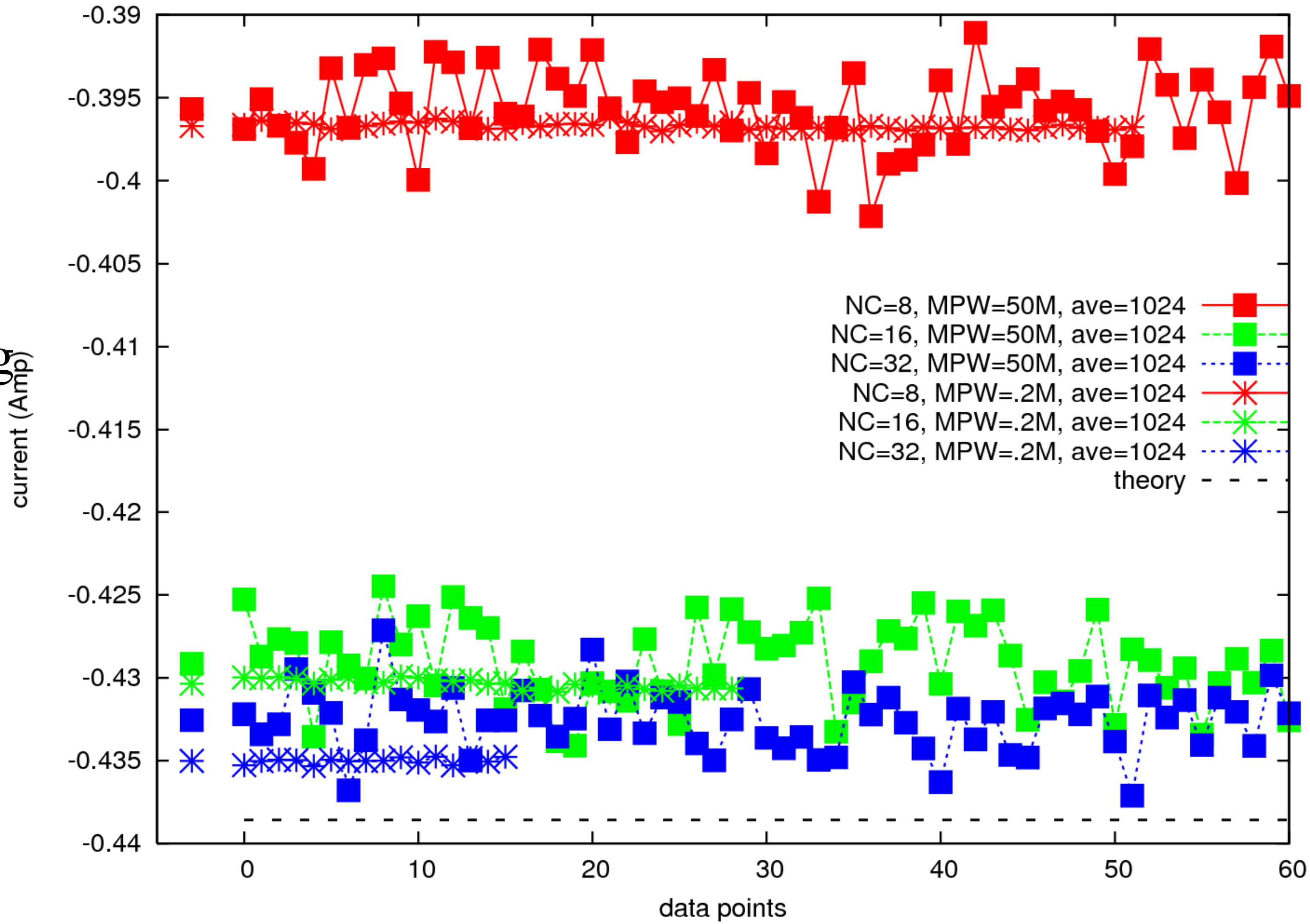
Product of particles and length of average results in the same "noise"

Simulations with more particles result in better result



Number of Particles and Average Convergence

If you can afford enough particles and/or long enough averages the stochastic nature can be minimized



Estimation of Parameters

Moments of a general distribution is a follows

$$\hat{\mu} = \bar{x} \equiv \frac{1}{N}\sum_{i=1}^{N} x_i, \quad \hat{\sigma}^2 \equiv \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2$$

Estimation of the mean is distributed normally (in the limit)

$$\hat{\mu} \sim \mathcal{N}(\mu, \frac{\sigma^2}{N})$$

$\mathcal{N}(\mu, \sigma^2)$ is a normal distribution with a mean μ and variance σ^2

For a given time series this leads to an estimation of the difference between the **estimated parameter and the true parameter**

$$\sqrt{N}(\hat{\mu} - \mu) \rightarrow \mathcal{N}(0, \sigma^2).$$

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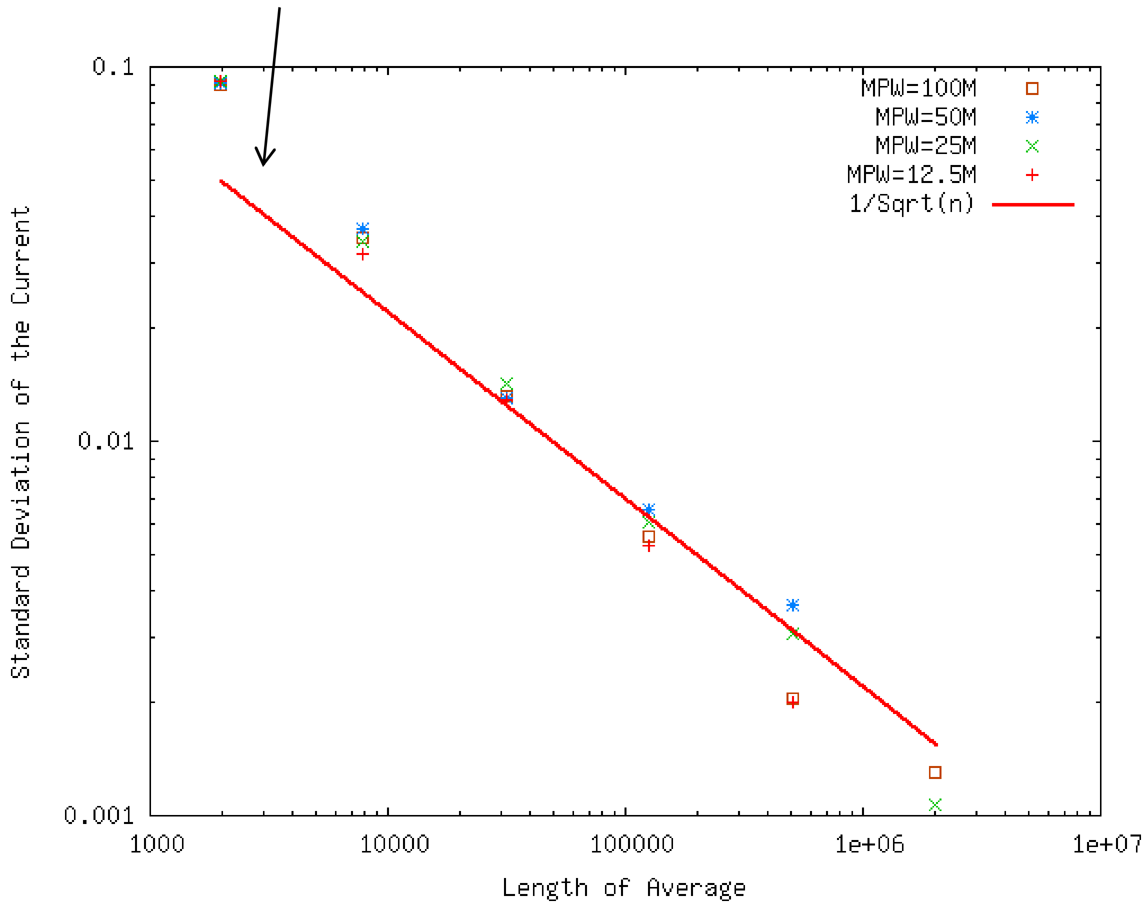
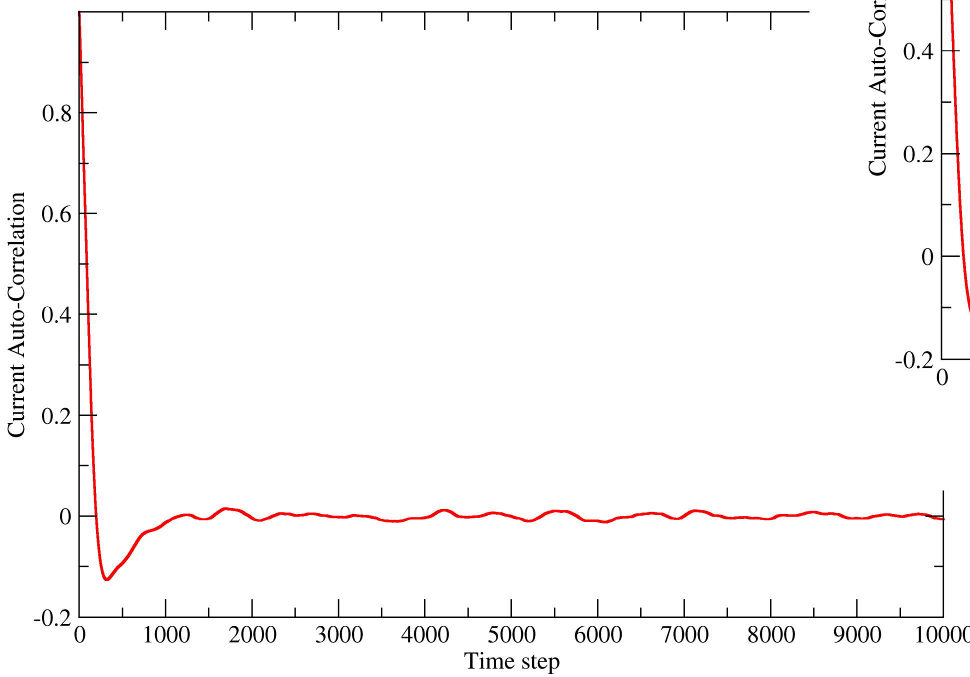
Error Estimation of the Mean

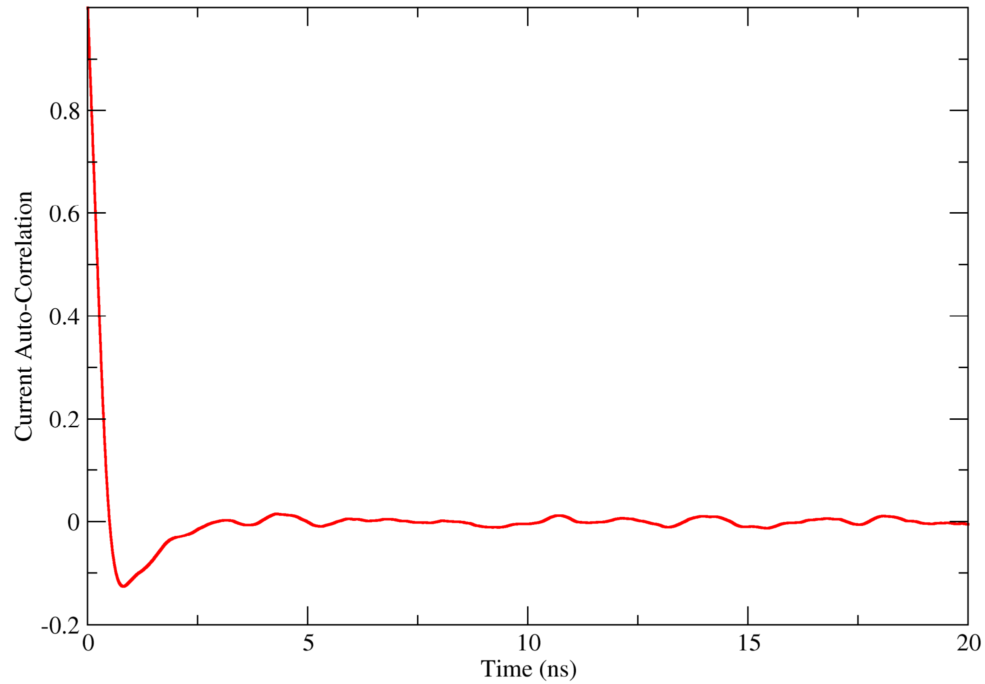
Short time correlation



Standard deviation scaled by the ratio of the square root of the macro particles

Correlation of Time Series





Two Variations of Richardson Extrapolation

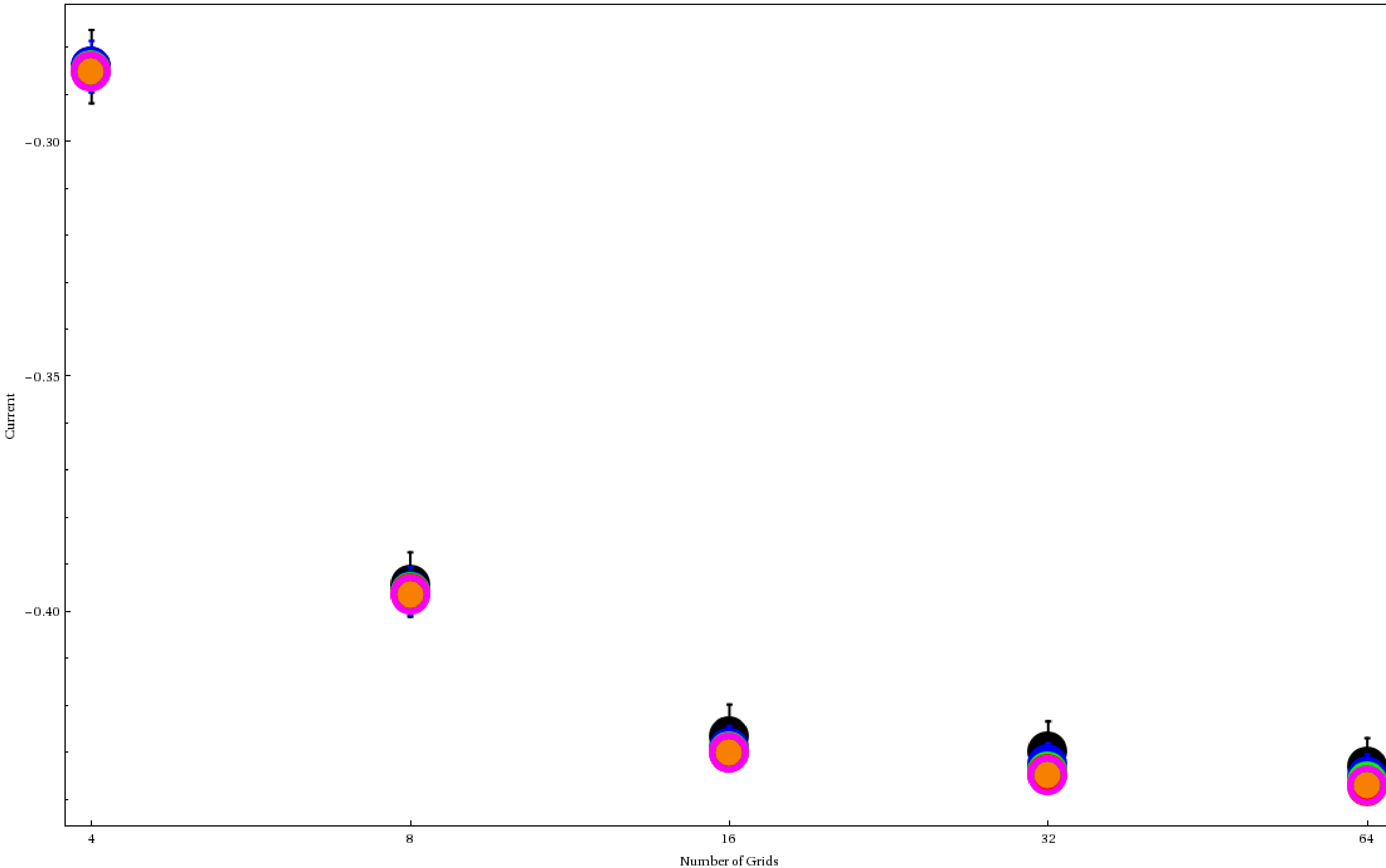
1. Weight the points by $1/\Delta y^2$; Δy is the uncertainty
2. Use all the points that would go into the uncertainty calculation

Same set of data for both fits:

NC=4, 8, 16, 32, 64

MPW=100M, 50M, 25M, … 390K, 195K, 97.7K

Data with Error Bars



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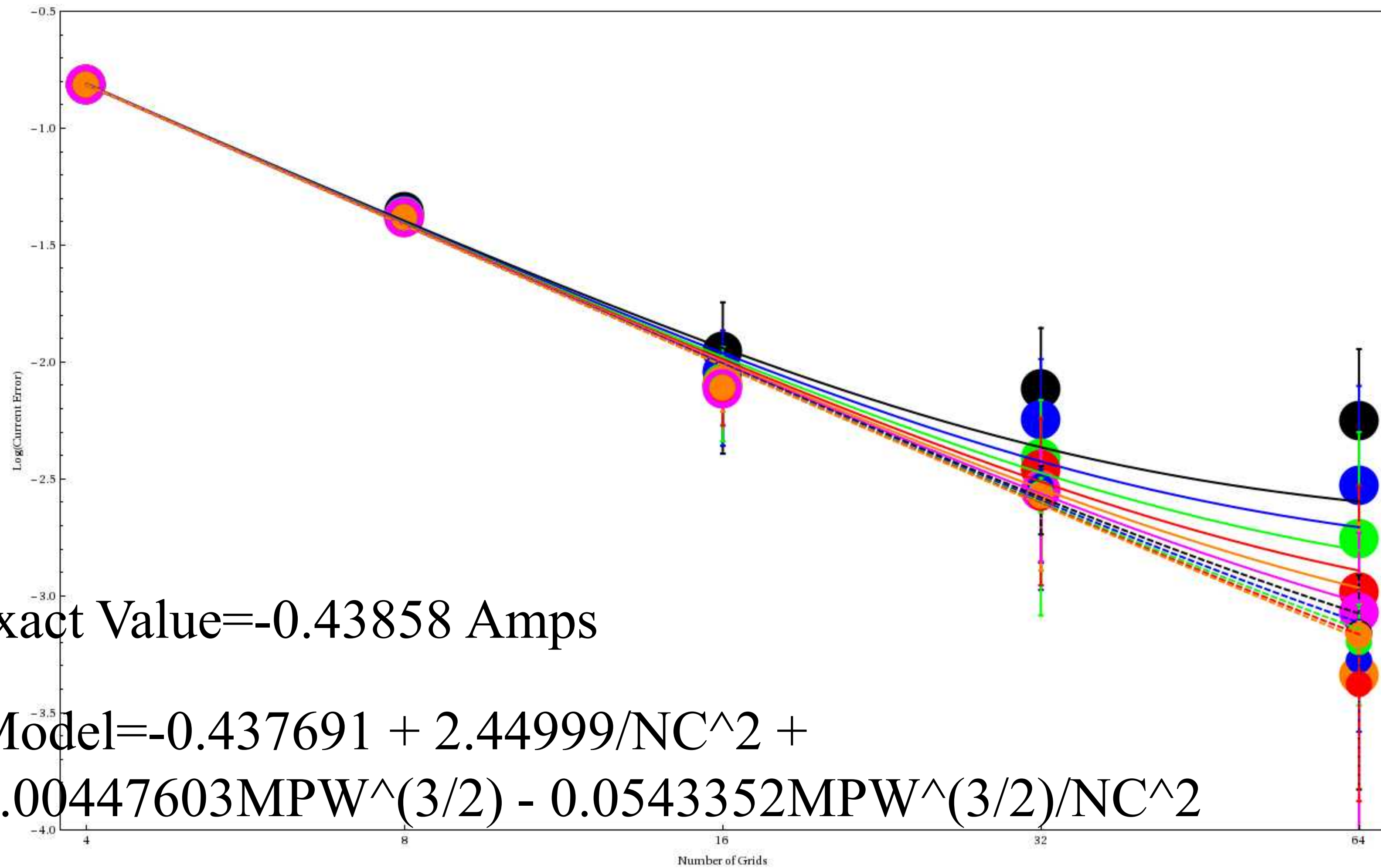
Data with Richardson Extrapolation



Exact Value=-0.43858 Amps

Model=-0.437691 + 2.44999/NC^2 + 0.00447603MPW^(3/2) - 0.0543352MPW^(3/2)/NC^2

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Model Difference (Expected Convergence Rates)

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Exact Value=-0.43858 Amps

Model=-0.437691 + 2.44999/NC^2 + 0.00447603MPW^(3/2) - 0.0543352MPW^(3/2)/NC^2

CI=±0.01

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Model Difference (Observed Convergence Rates)

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Exact Value=-0.43858 Amps

Model=-0.438395 + 2.19054/NC^1.91825 + 0.00409125MPW^1.55357 - 0.0410527MPW^1.55357/(NC^1.91825)

CI=±0.01

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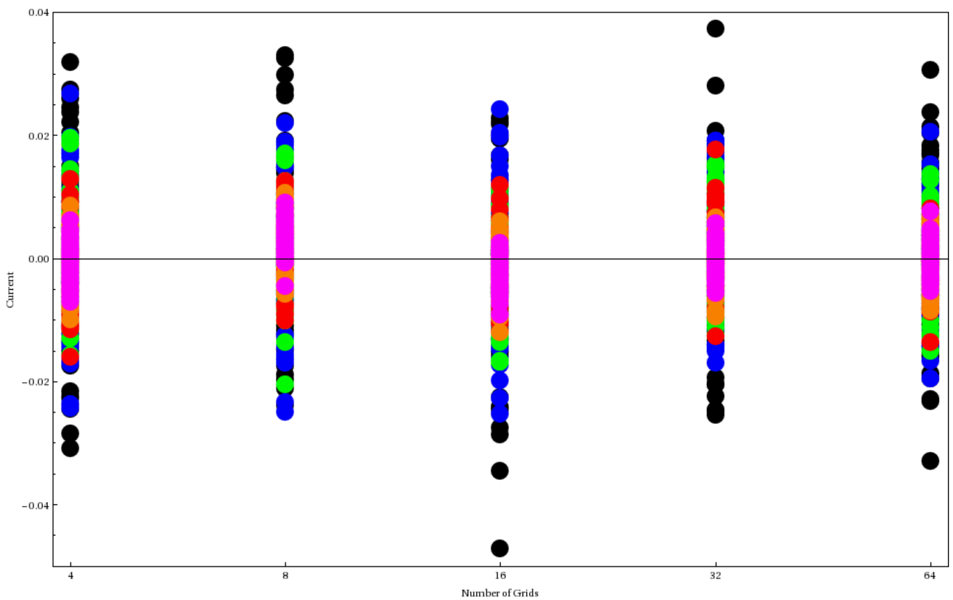
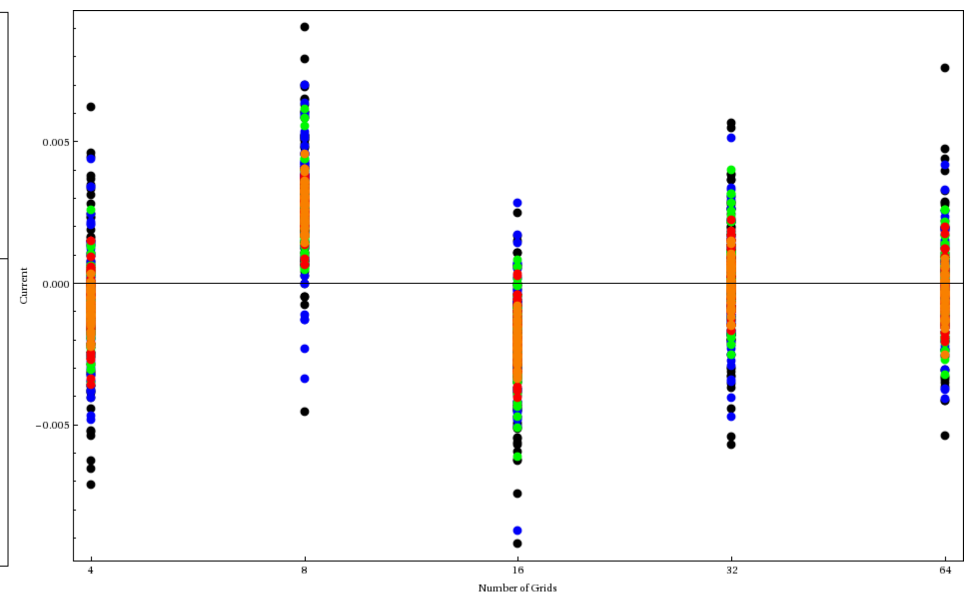
Model Difference (Expected Convergence Rates)

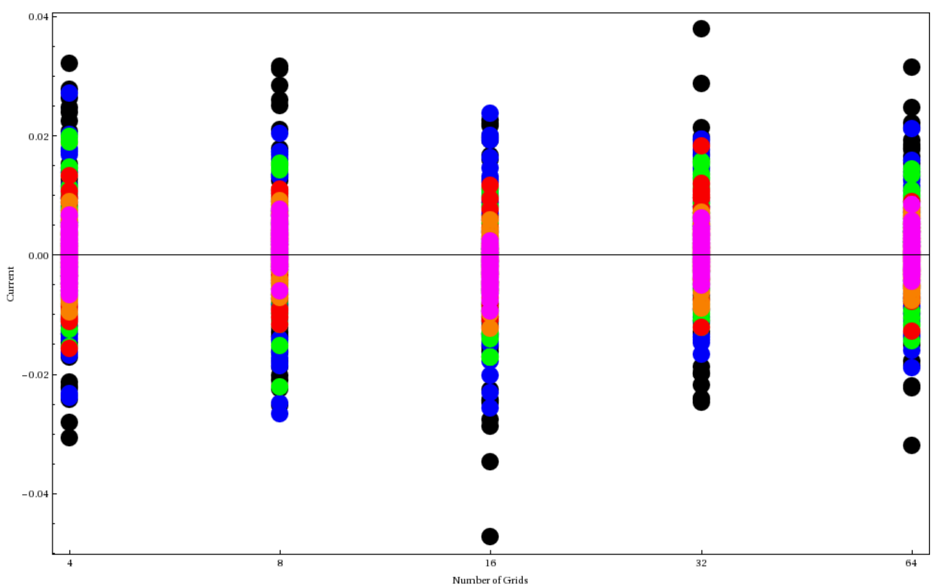


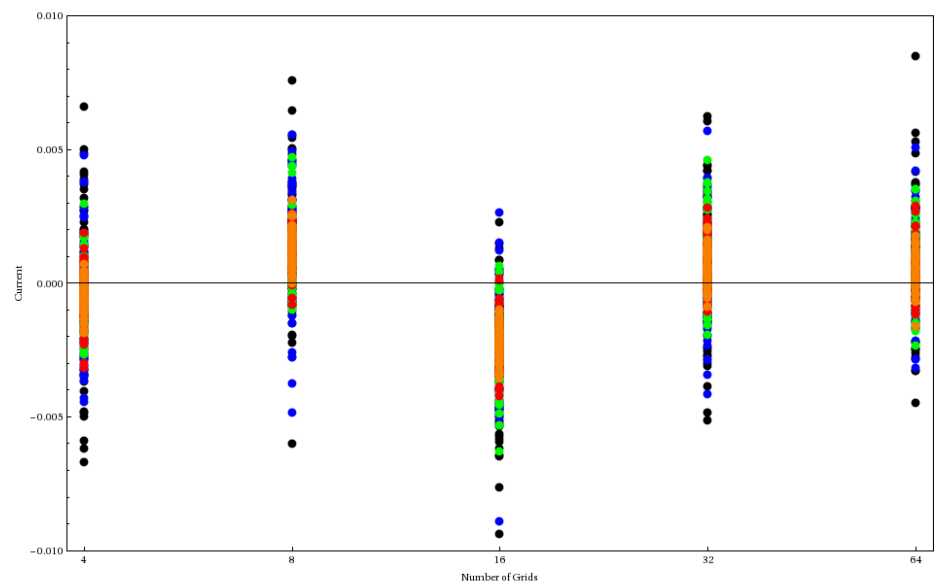


Exact Value=-0.43858 Amps
Model=-0.437541 + 2.45009/NC^2 + 0.0060602MPW^(3/2) – 0.104671MPW^(3/2)/NC^2

CI=±0.03

Model Difference (Observed Convergence Rates)





Exact Value=-0.43858 Amps

Model=$-0.438619 + 2.18509/NC^{1.91418} + 0.00607912MPW^{1.3184} - 0.0920017MPW^{1.3184}/(NC^{1.91418})$

CI=±0.04

Conclusions

- Both Richardson Extrapolation methods bound the theoretical results
  - Robust CI because it is based on how well the model matches the simulation results

Work in progress

- Work on optimized regression for RE
  - Better choices of MPW and NC
- Look at spatial convergence
- Longer time line
  - Develop a time dependent verification problem

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