Monte Carlo Investigations of Electron Decoherence due to Phonons

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The Considered Problem Domain

States of quantum computation

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \qquad\qquad |\alpha|^2 + |\beta|^2 = 1$$

Classically: in either in state 0 or in state 1

Quantum setting: in all of the states at the same time

State Selection

States chosen as one-dimensional Gaußian wave-packets

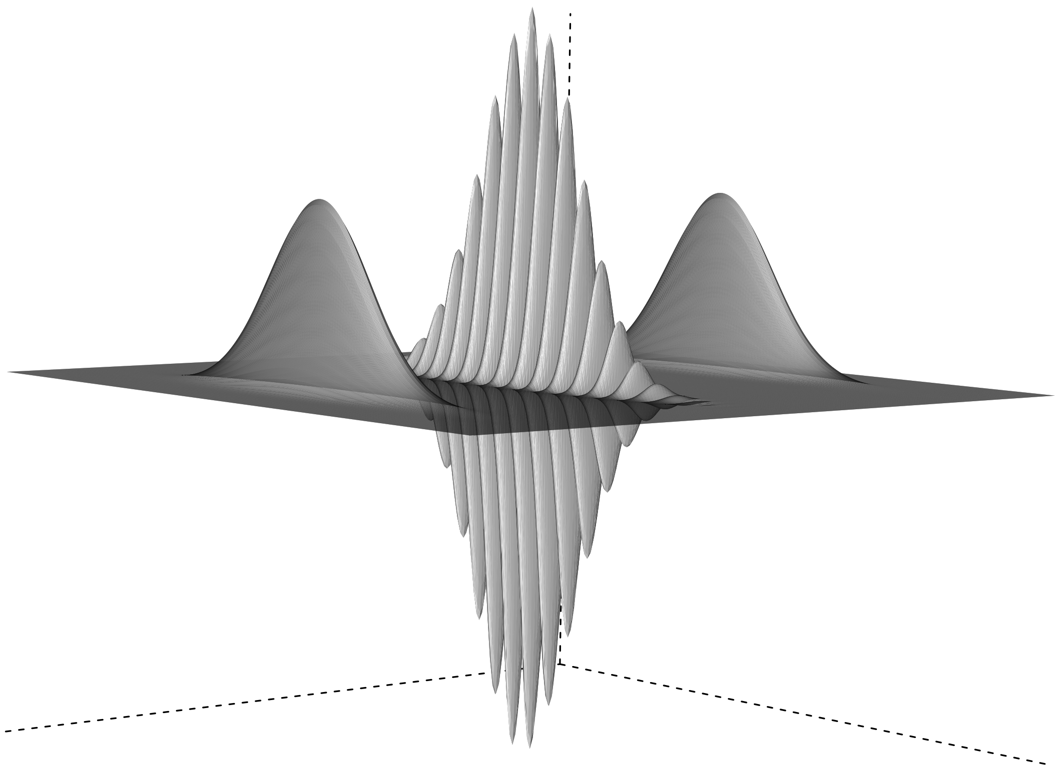
$$|0\rangle, |1\rangle = \mathrm{e}^{\frac{-(x\pm a)^2}{2\sigma^2}} \mathrm{e}^{\imath bx}$$

Corresponding phase space Wigner function

$$\mathrm{e}^{-(k_\mathrm{x}-b)^2\sigma^2} \left[\mathrm{e}^{-\frac{(x-a)^2}{\sigma^2}} + \mathrm{e}^{-\frac{(x+a)^2}{\sigma^2}} + \color{red}{\mathrm{e}^{-\frac{x^2}{\sigma^2}} \cos\left((k_\mathrm{x} - b)2a\right)} \right]$$

An Image from Phase Space

Oscillations of the Wigner function are indications of quantum nature



Evolution in Phase Space

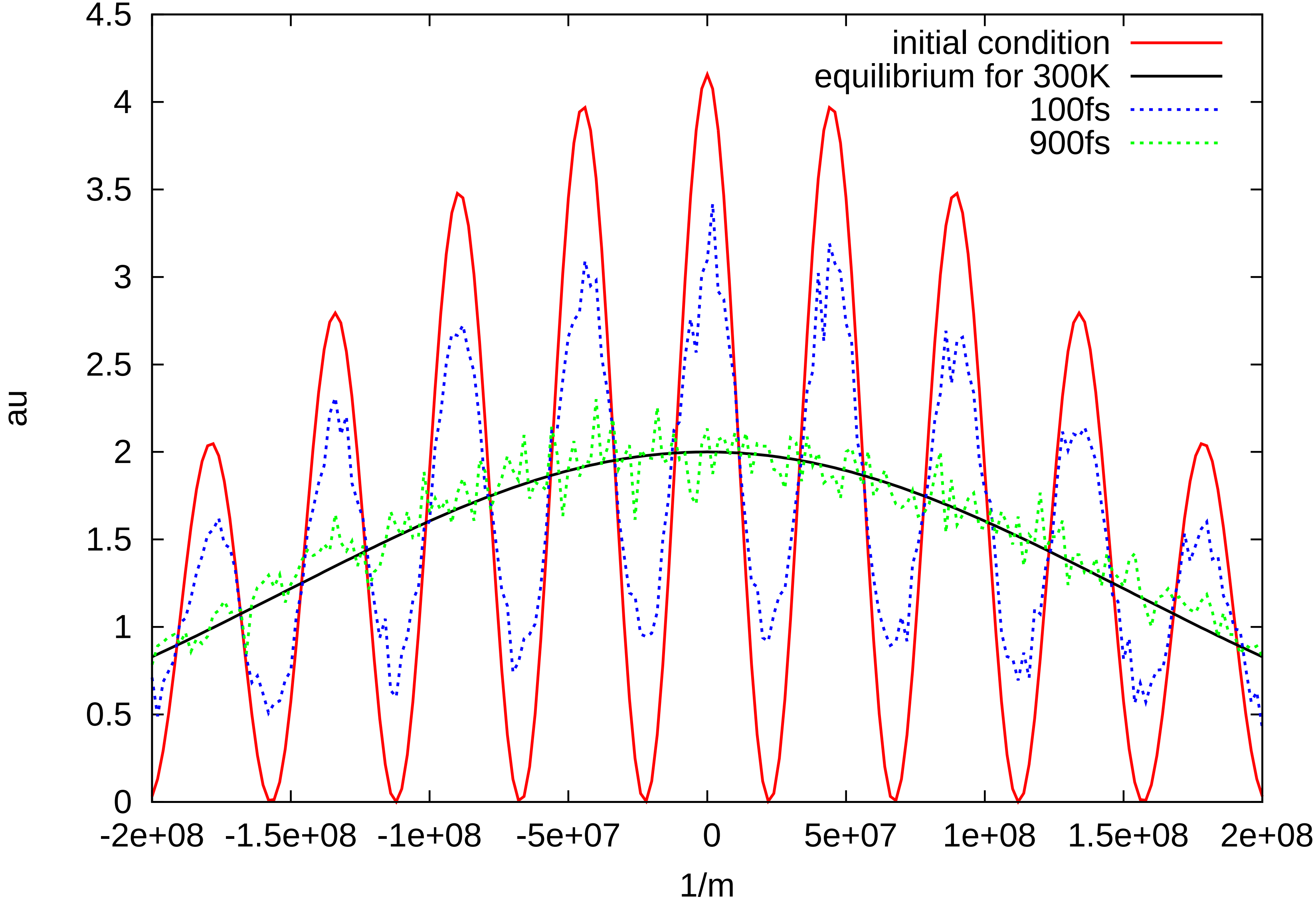
Phase breaking evolution of Wigner-Boltzmann type equation

$$\left(\frac{\partial}{\partial t} + \frac{\hbar k_{\mathrm{x}}}{m}\frac{\partial}{\partial x}\right) f_{\mathrm{w}}(x,\mathbf{k},t) = \int d\mathbf{k}' f_{\mathrm{w}}(x,\mathbf{k}',t) S(\mathbf{k}',\mathbf{k}) - f_{\mathrm{w}}(x,\mathbf{k},t)\lambda(\mathbf{k})$$

This evolution pushes towards thermal equilibrium

Classic Configuration due to Scattering

Quantum information dissipates to thermal equilibrium



Algorithm A

A single grid is used for estimators as well as particle generation

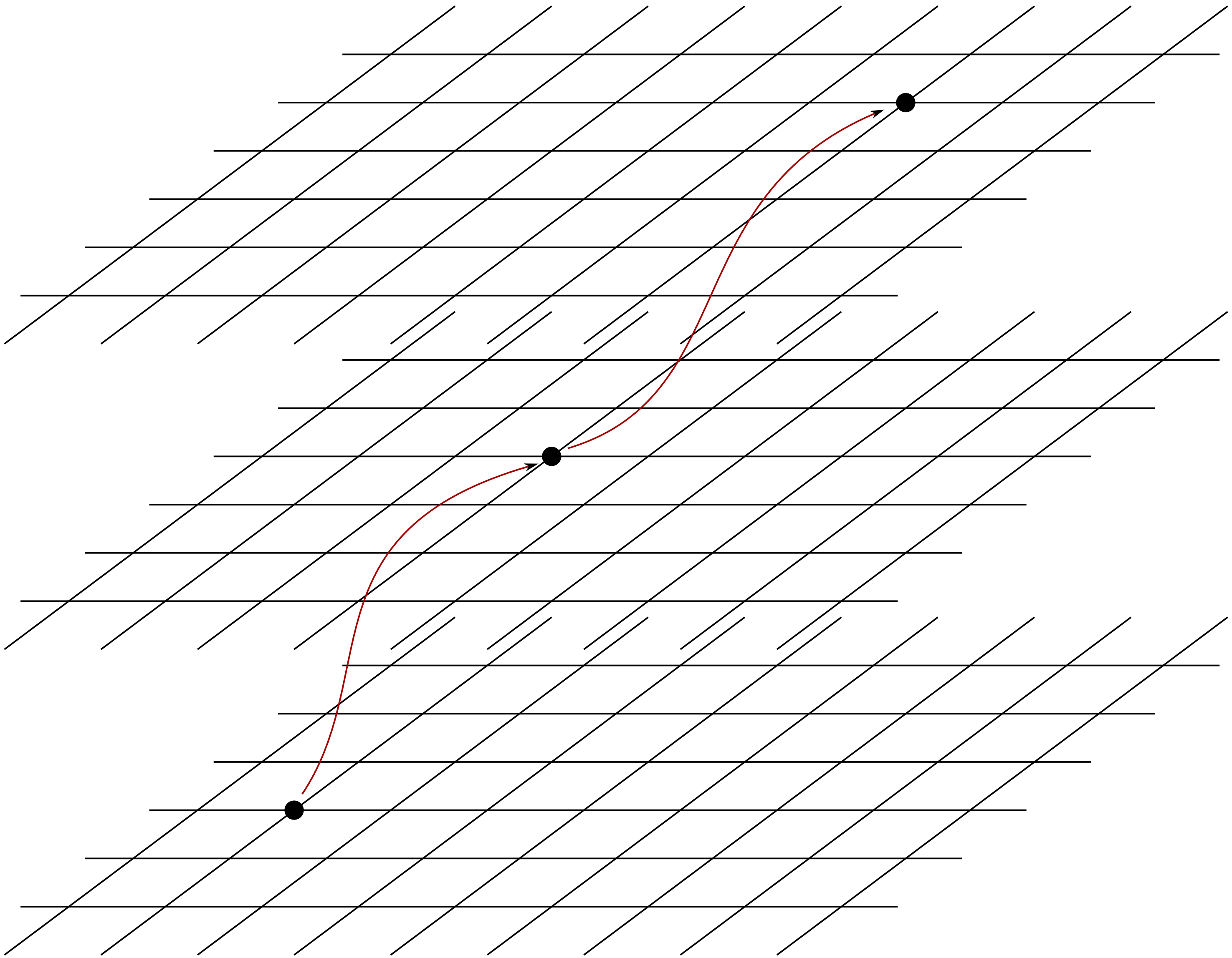
Each particle carries a weight corresponding to the initial configuration

Each generated particle is evolved through all of the desired time steps

Memory requirements:

$$\mathrm{sizeof}(estimator) \times (\#time\ steps) + \mathrm{sizeof}(particle\ state)$$

Algorithm A



Algorithm B

A single grid is used for estimators as well as particle generation

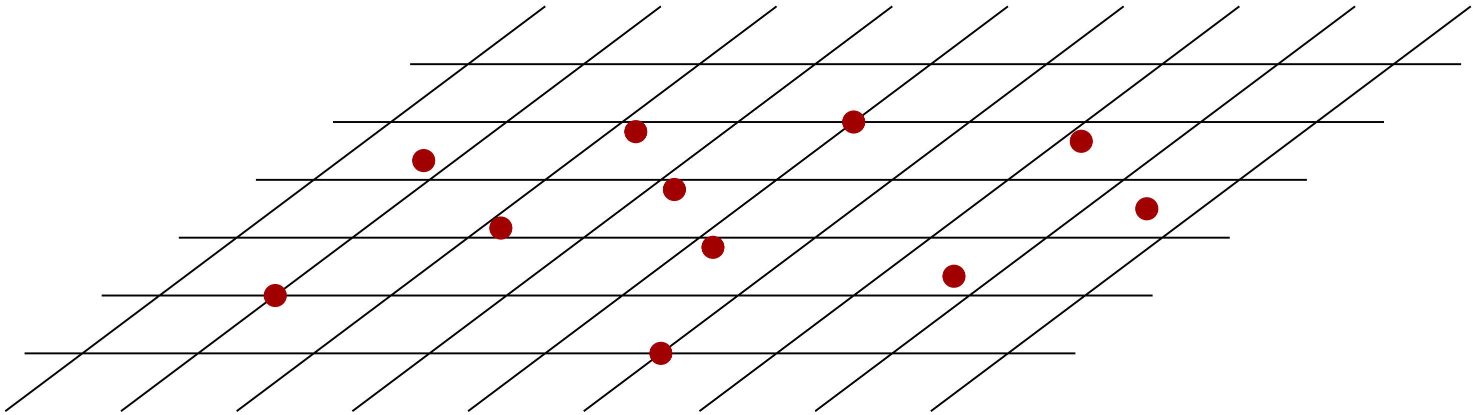
Each particle carries a weight corresponding to the initial configuration

Particles are evolved as an ensemble

Memory requirements:

$$\mathrm{sizeof}(particle\ state) \times (\#particles) + \mathrm{sizeof}(estimator)$$

Algorithm B



Algorithm C

A grid is used for the estimators

A cell structure is used to store particle weights

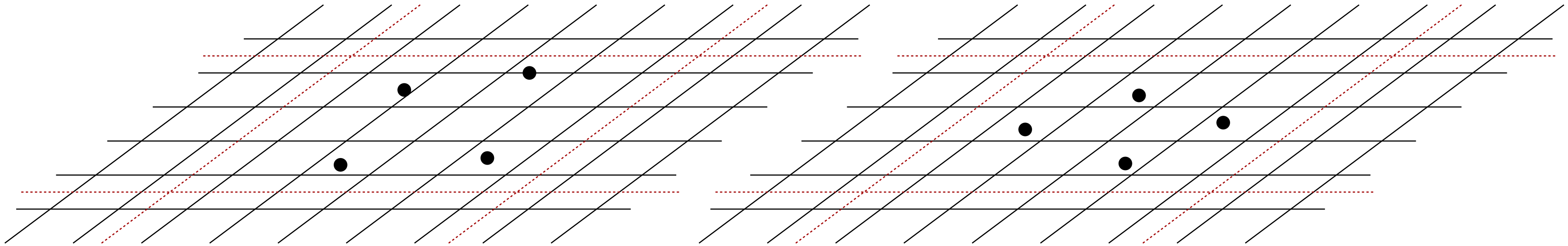
Particles are randomly generated from each of the cells

Estimates are recorded against the estimator grid

Memory requirements:

$$
\begin{aligned}
(\#cells) \times \mathrm{sizeof}(weight) &+ \mathrm{sizeof}(particle\ state) \\
&+ \mathrm{sizeof}(estimator)
\end{aligned}
$$

Algorithm C



Setup of the Comparison

Estimator grid of 4000×3000 points

Algorithms A and B give matching results

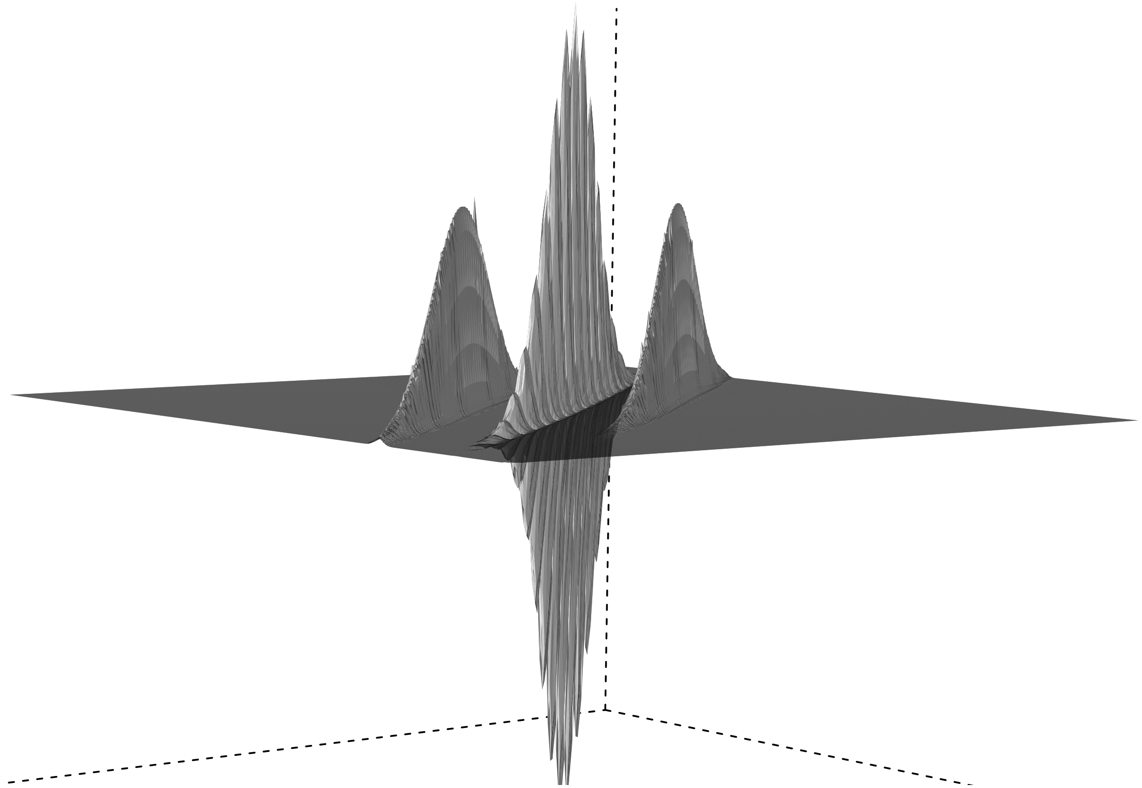
Algorithm C applied with different cell sizes

100 time steps

Algorithm	Memory Requirement
A	8.84 GiB
B	139.14 MiB
C (fine)	183.11 MiB
C (coarse)	92.47 MiB

Coherent Evolution

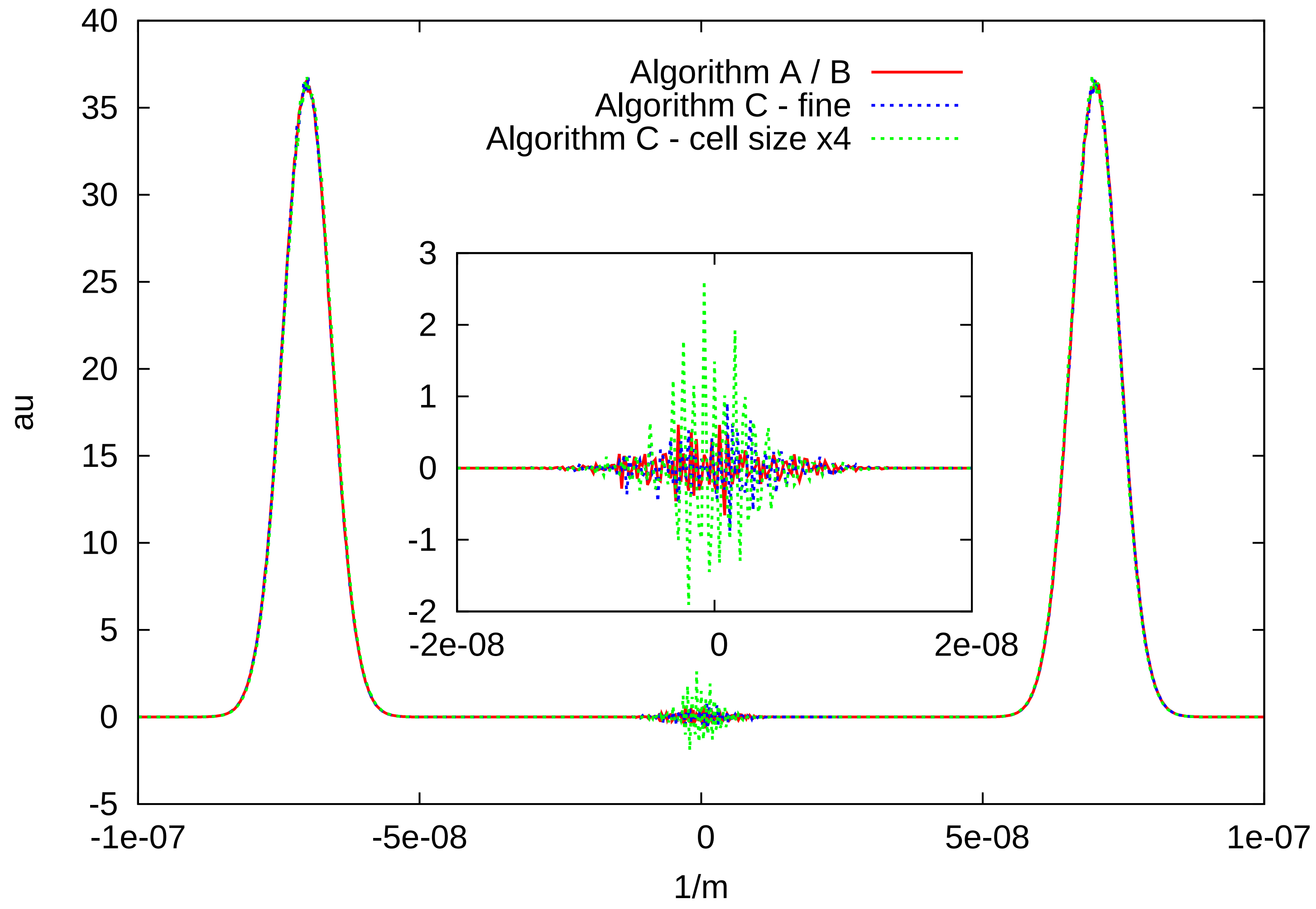
Phase space distribution after $900\mathrm{fs}$ of coherent evolution



The quantum characteristics are preserved

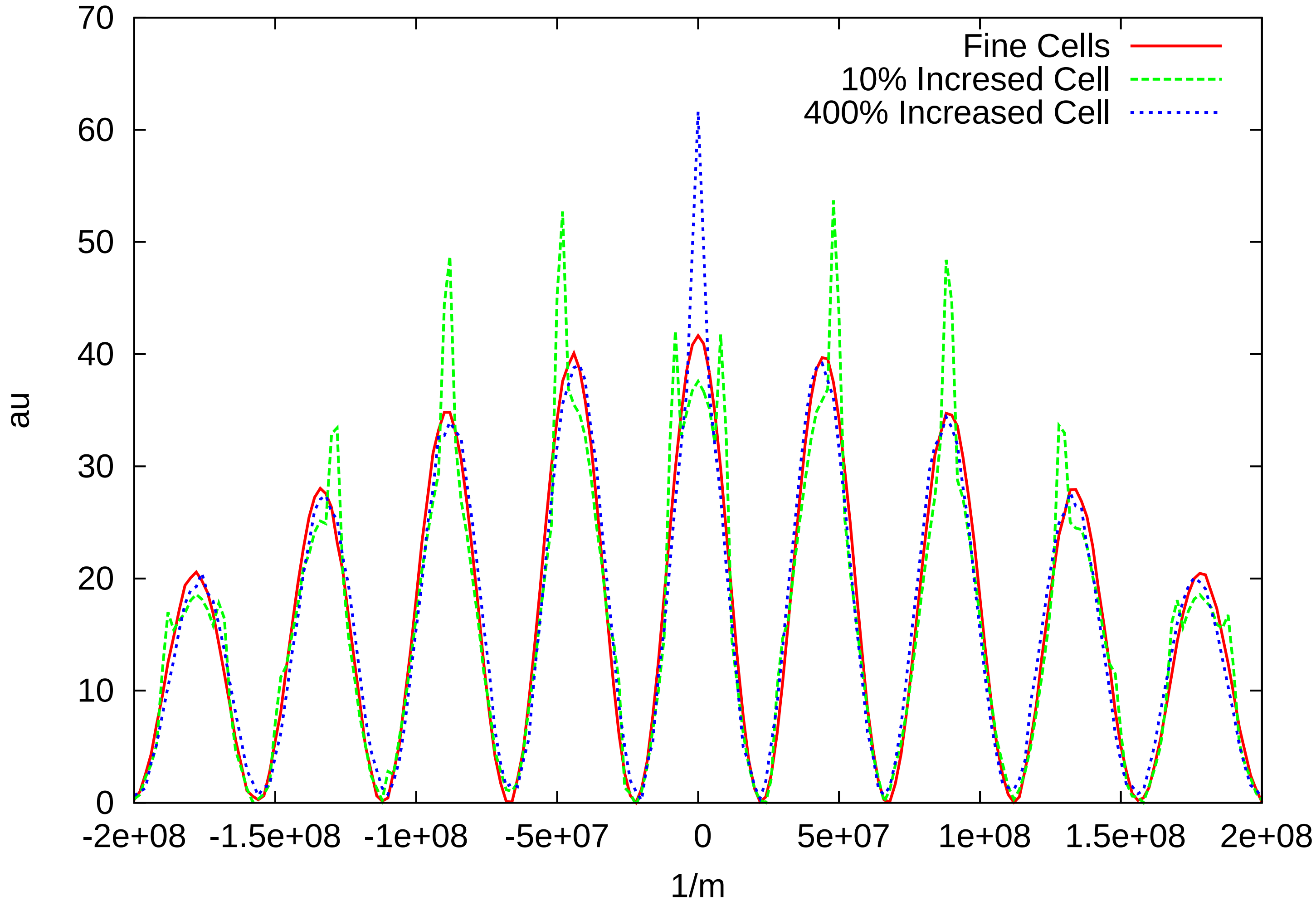
Coherent Evolution

Reconstruction of densities after a single time step



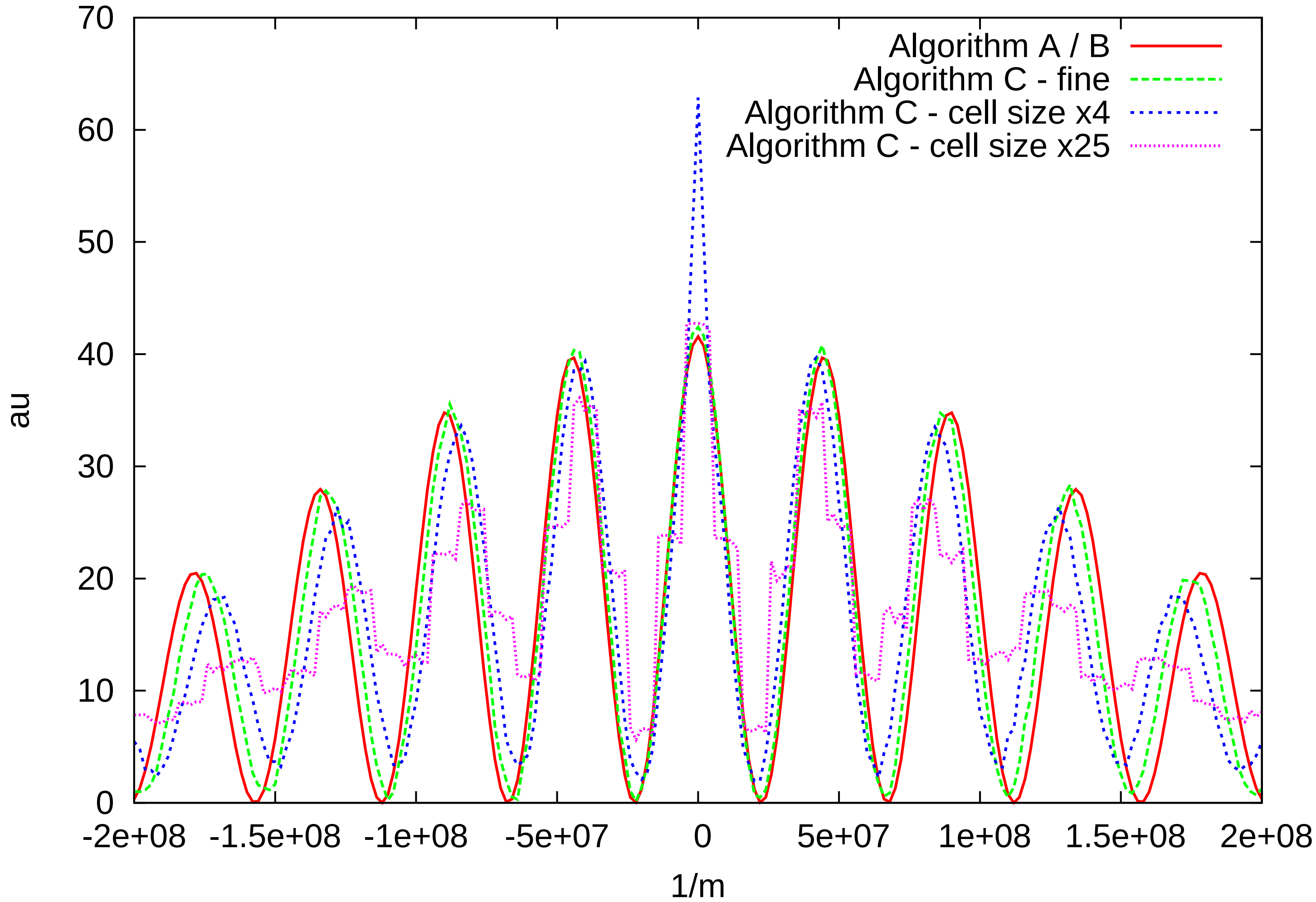
Coherent Evolution

Momentum distribution after $10\mathrm{fs}$



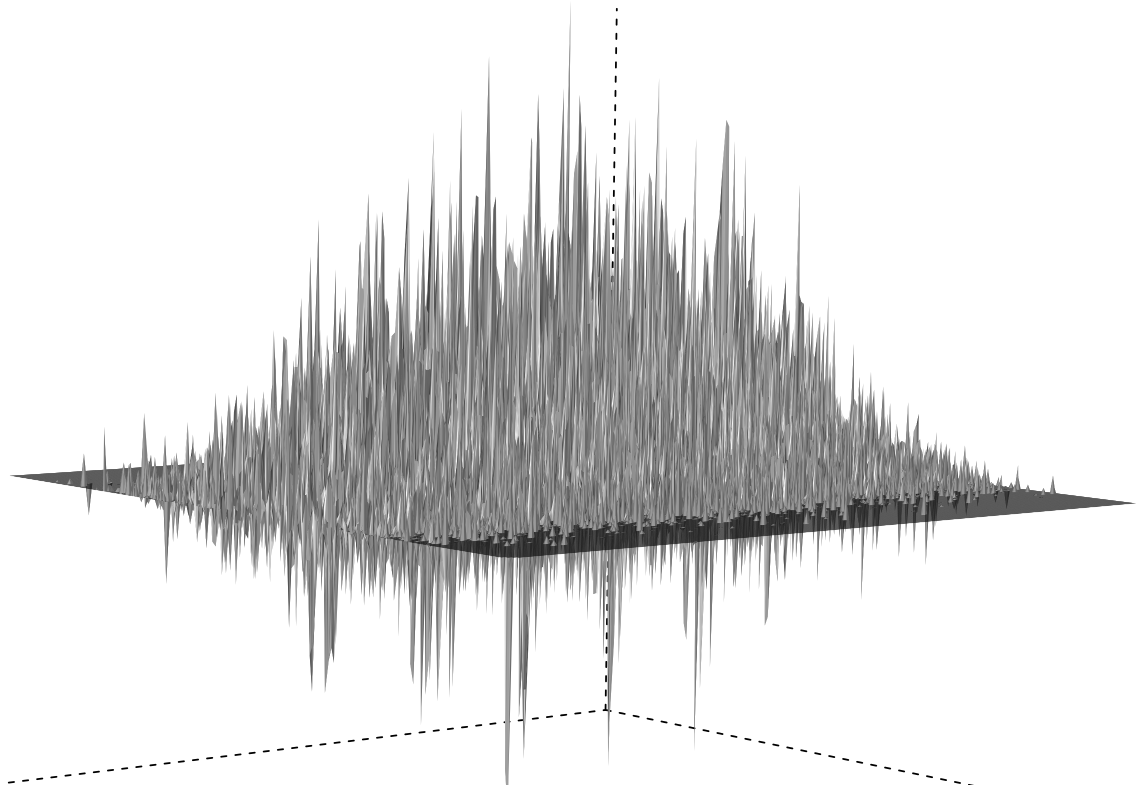
Coherent Evolution

Momentum distribution after $700\mathrm{fs}$



Phase Breaking Evolution

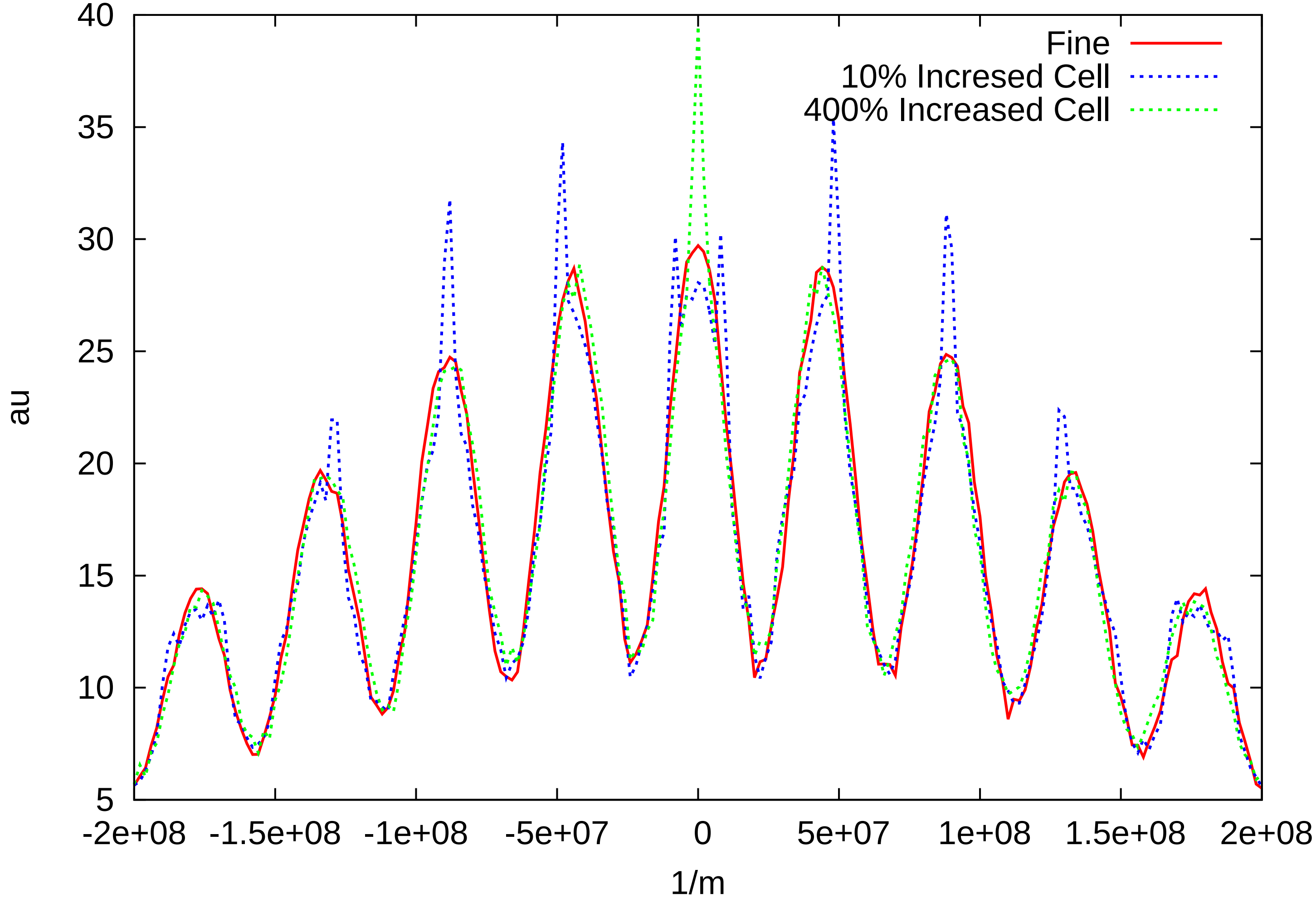
Phase space distribution after $900\mathrm{fs}$ of phase breaking evolution



The quantum characteristics are destroyed

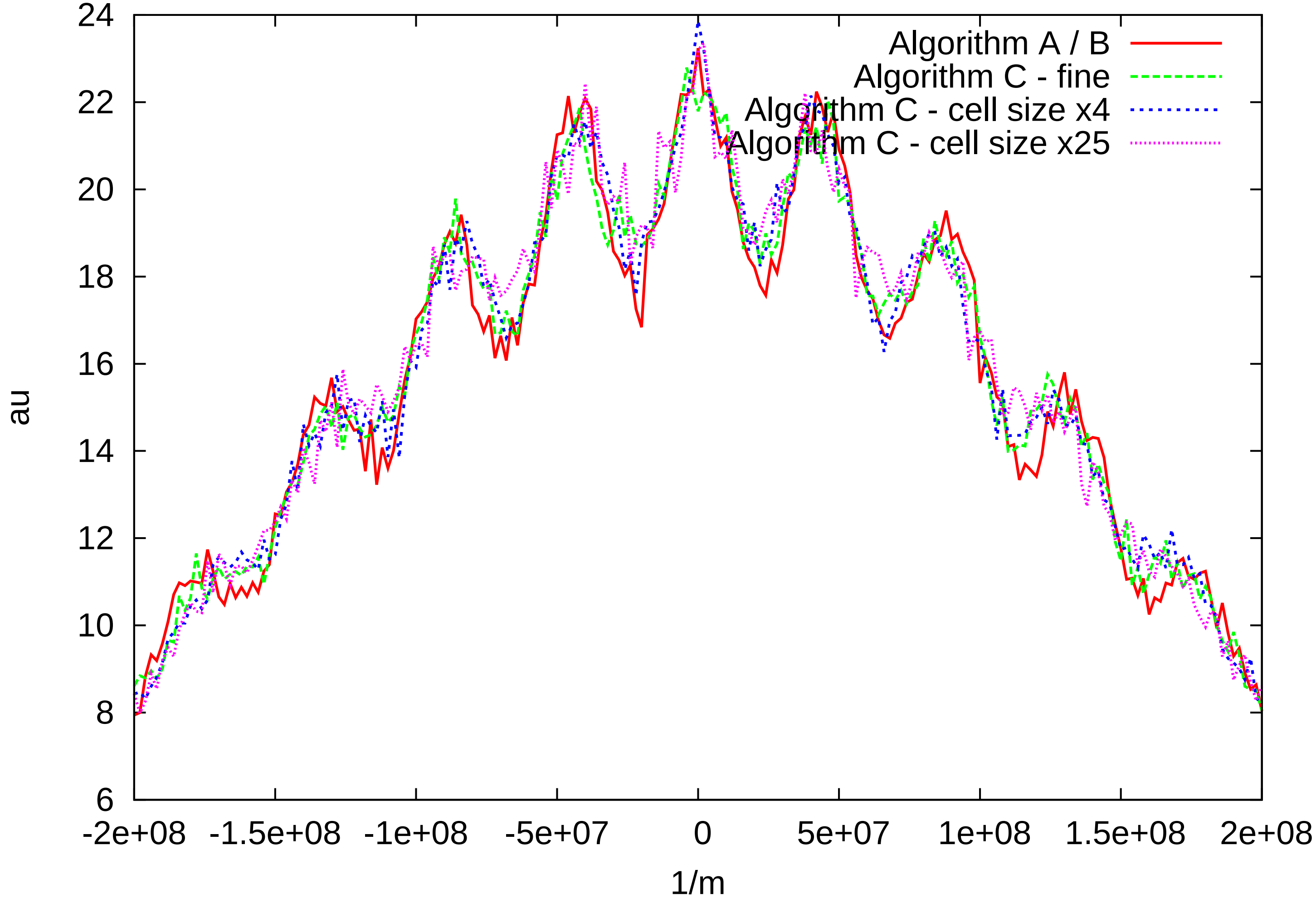
Phase Breaking Evolution – First Moments

Momentum distribution after $10\mathrm{fs}$



Phase Breaking Evolution

Momentum distribution after $300\mathrm{fs}$



Conclusion

- Three different algorithm for the evolution of a coherent state
- Algorithms A and B give agreeing results
- Cell based algorithm can produce agreement
  - Sensitivity to cell size
  - Sensitivity to cell and estimator placement
- Phase breaking effects dominate numerical effects

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Thank you for your attention

Something Completely Different

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The Larch