IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

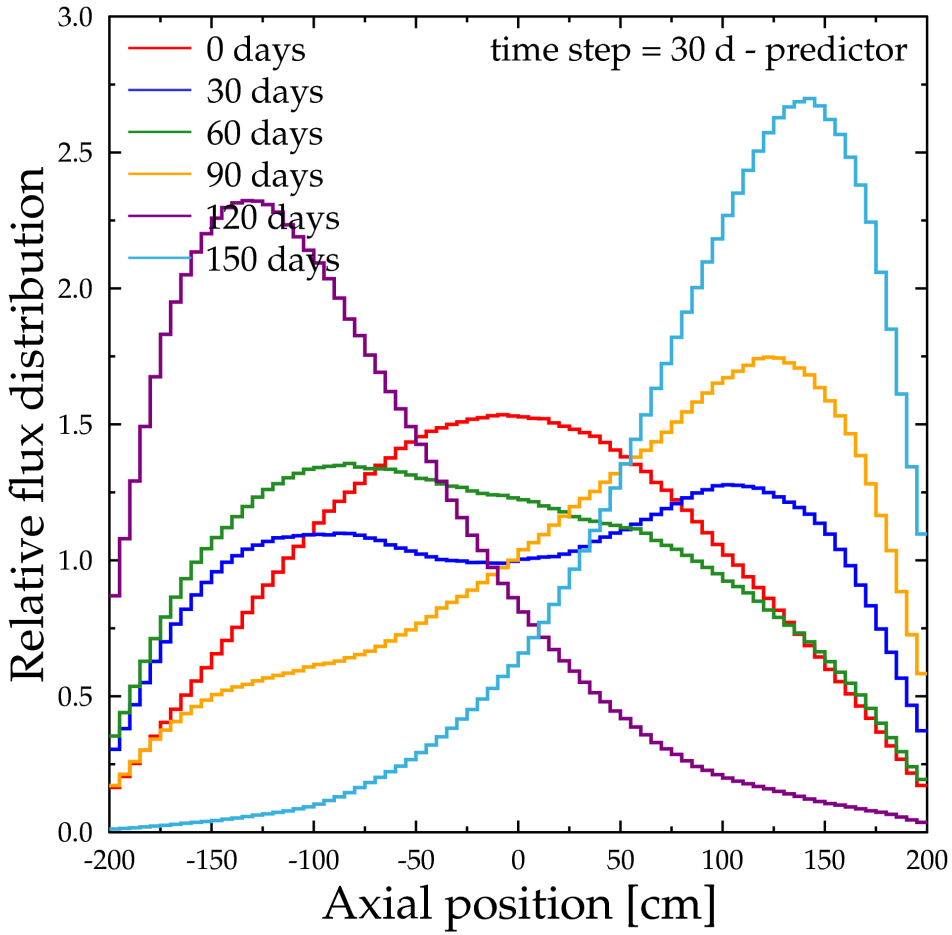
Convergence issues in Best-estimate Monte Carlo Depletion Calculations

This presentation…

- … is a detailed version of NEA / Source Convergence Expert Group one (2009)
- … focuses on Monte Carlo issues when used in depletion calculations
- … is just the first step of a work in progress !

This presentation...

- **Motivated by this « strange » result (VESTA / MCNP non reflected rod)**



- Few words about Monte Carlo depletion calculations
- A first MC discrepancy benchmarking
- Proposal for extended benchmarking
- Some raising issues of Monte Carlo depletion calculations

Few words about Monte Carlo depletion calculations

- **Boltzmann Markov chain Monte Carlo solver (versus deterministic/mesh)**
  - Advantages
    - No geometry constraint or approximation (dimension or shape)
    - Built-in uncertainty estimation
    - Uncertainty control (over time of calculation)

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- **Boltzmann Markov chain Monte Carlo solver (versus deterministic/mesh)**
  - Advantages
    - No geometry constraint or approximation (dimension or shape)
    - Built-in uncertainty estimation
    - Uncertainty control (over time of calculation)
  - Disadvantages
    - CPU cost
    - Markov chain burn-in
    - Some estimators are biased (fluxes)
    - Not easy to parallelize
    - Not easy to get O/I sensitivity vectors

Few words about Monte Carlo depletion calculations

- **Development trends of MC depletion interfaces**
  - MONTEBURNS (MCNP / ORIGEN)
  - ALEPH (MCNP / ORIGEN)
  - VESTA (MCNP|MORET / ORIGEN|PHOENIX)
  - SERPENT (PSG / ...)
  - MOCA
  - …

Few words about Monte Carlo depletion calculations

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  - MOCA
  - …
- **Only Best-Estimate approaches**
  - No MC discrepancy control or estimation
  - No ND uncertainties propagation

A first MC discrepancy benchmarking

- **MC discrepancy**

  Monte Carlo neutron simulation provides fluxes or reaction rates
  which mean is used as best estimate value
  => **20** different initial random seed lead to different composition output

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- **Few words about tools involved**
  - VESTA – MC depletion interface
    - Monte Carlo code: MORET | MCNP
    - Depletion module: PHOENIX | ORIGEN

  (Soon) available at http://www.irsn.org/vesta & http://www.irsn.org/moret

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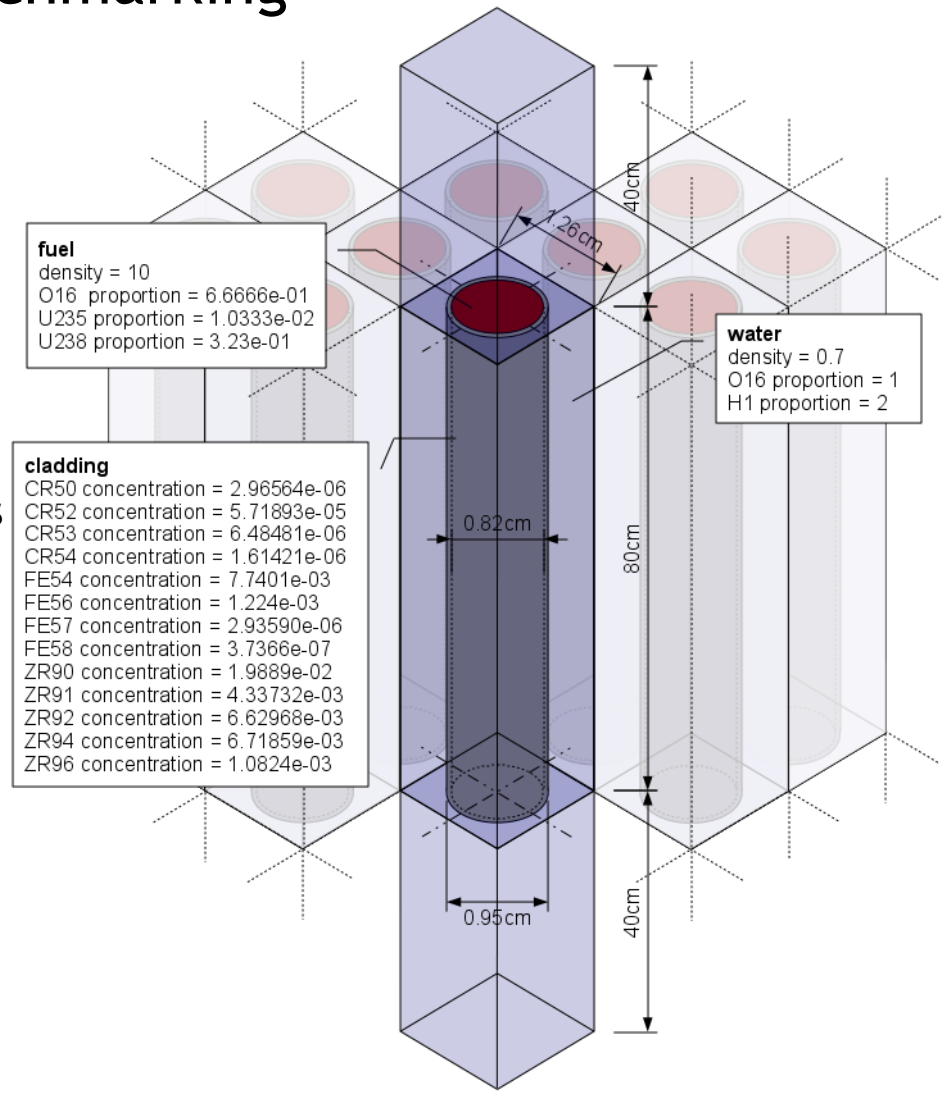
    (Soon) available at http://www.irsn.org/vesta & http://www.irsn.org/moret
  - PROMETHEE – grid for parametric calculation
    - Generic computing environment for any code
    - Efficiently parallel dispatch of calculations over all connected servers
    - User friendly front-end intended to be used for both day-to-day engineering or research
    - May embed algorithms for advanced computing tasks (uncertainty propagation, sensitivity analysis, optimization, calibration, ...)

    Freely available at http://www.irsn.org/promethee

A first MC discrepancy benchmarking

- **Infinite lattice of PWR rod**
  - Standard composition of fuel
  - Reduced height
  - Cladding
  - Infinite lattice modeled by reflection over water box faces XY, YZ, YZ



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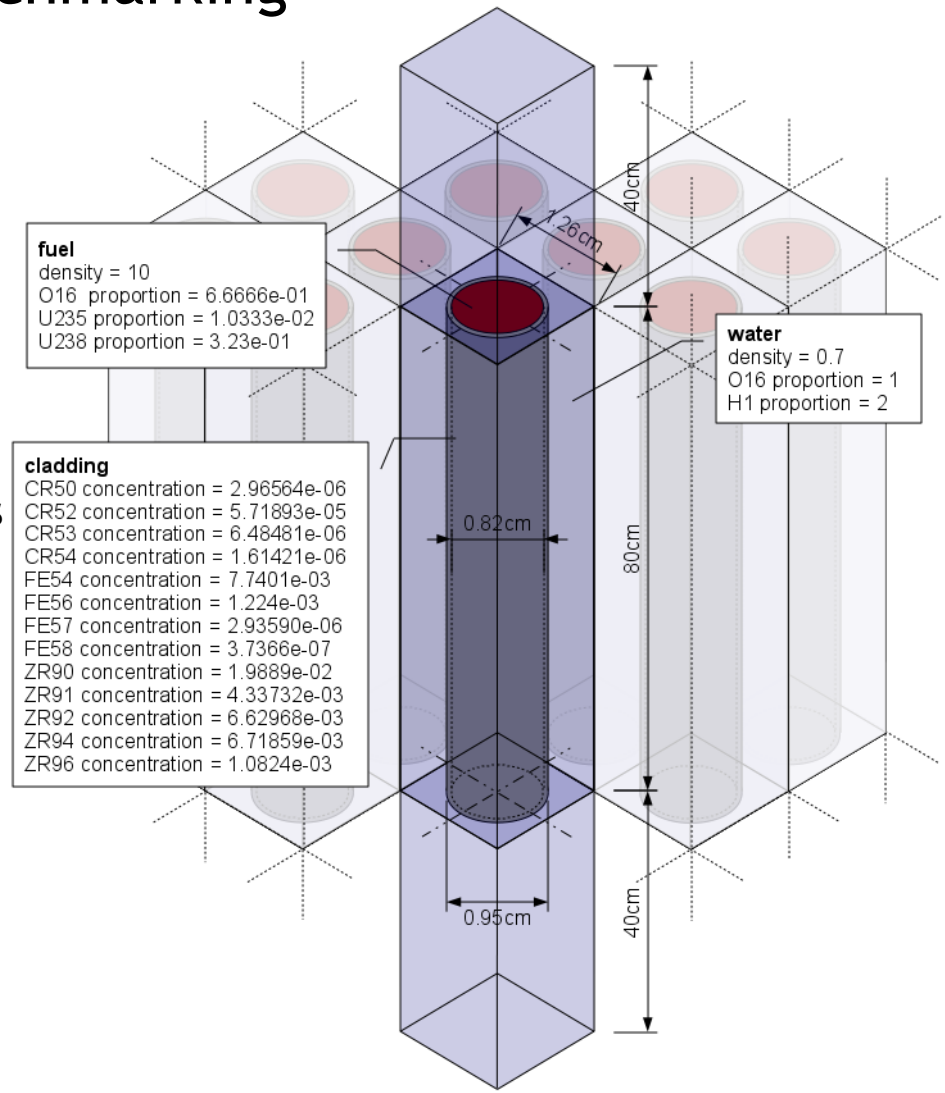
  - 20 days, constant power



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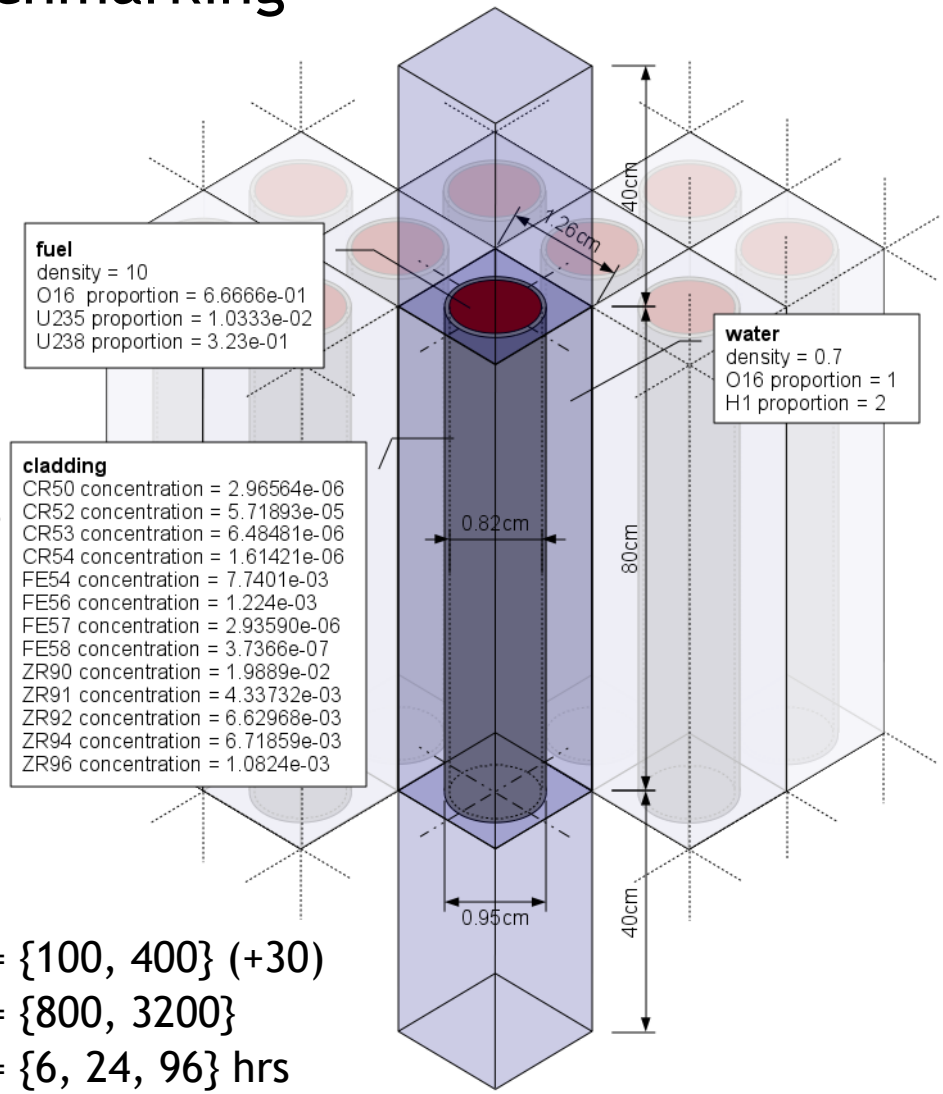
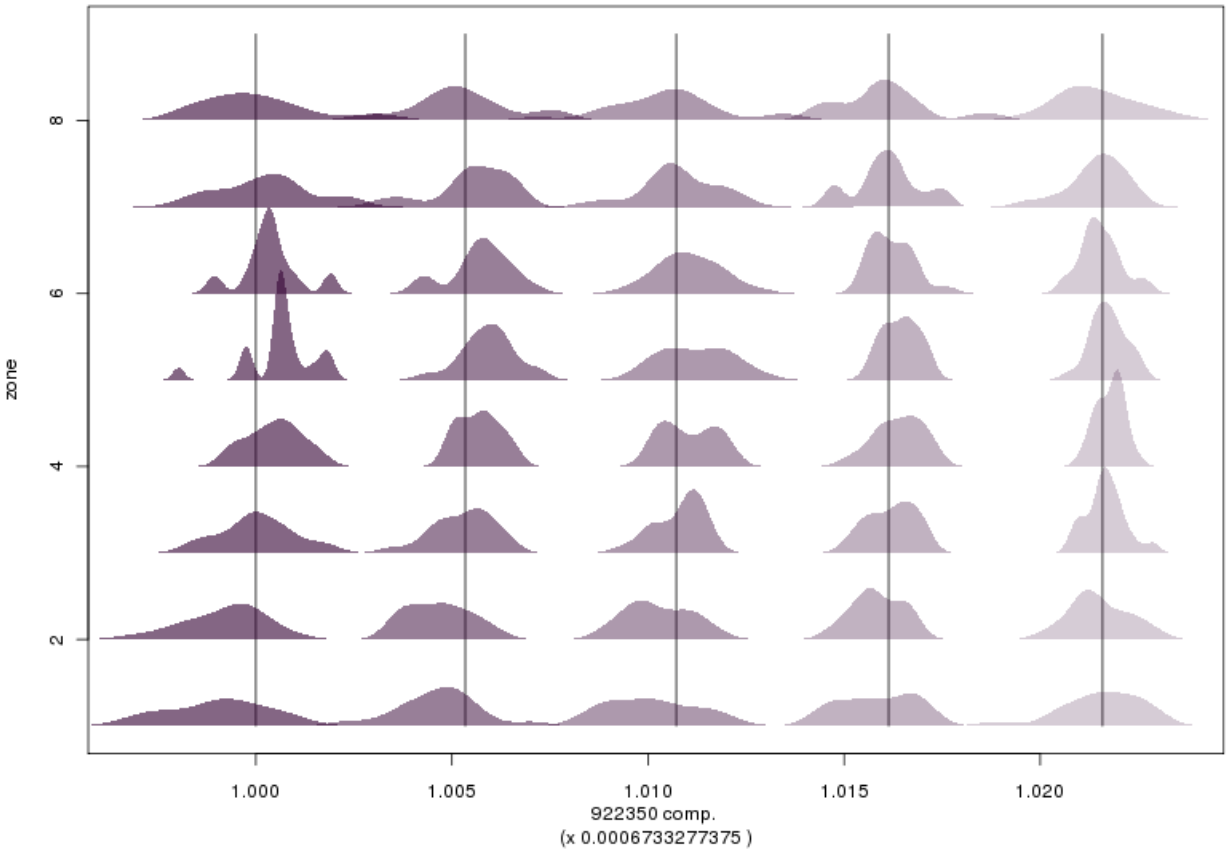
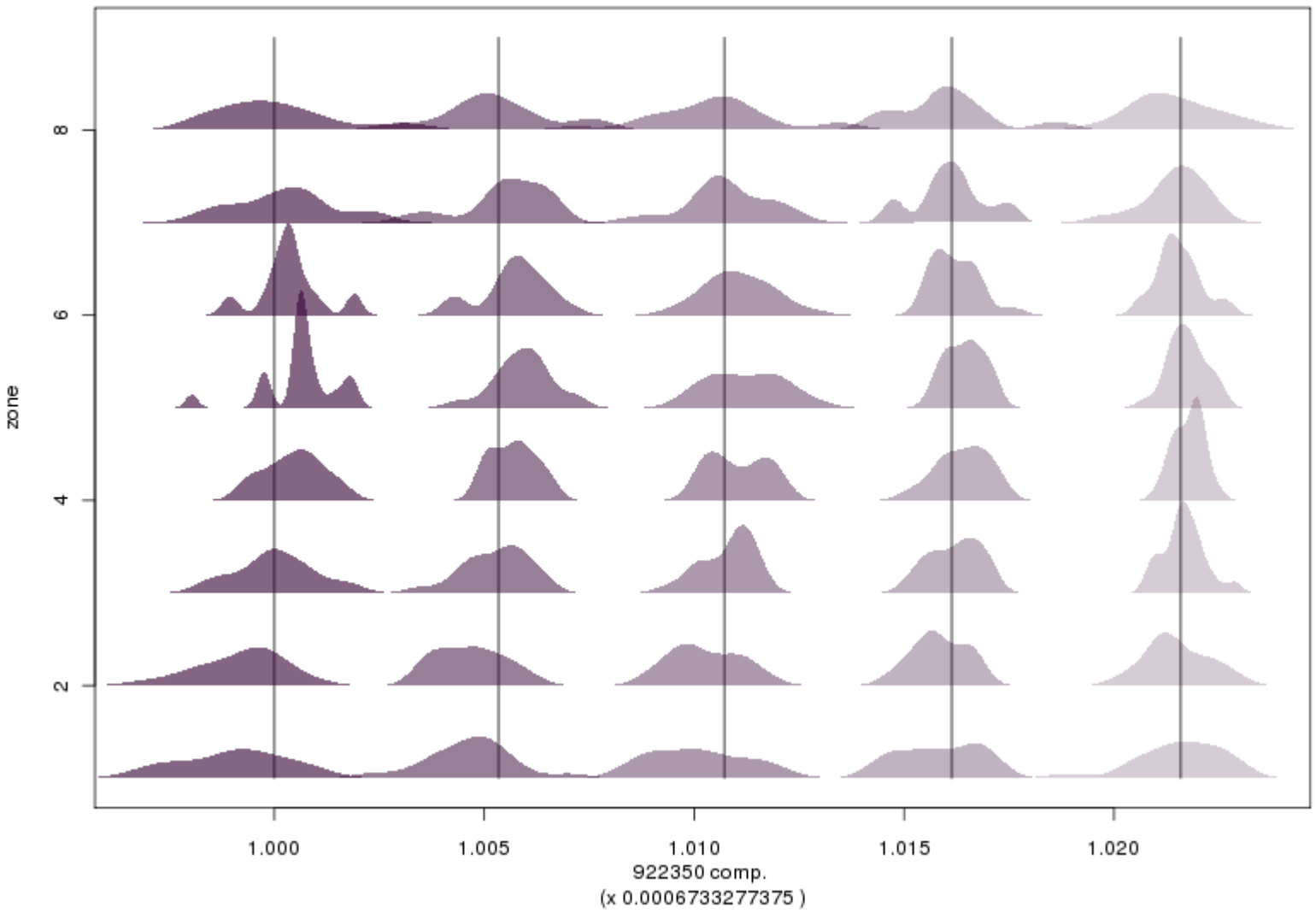
  - Focus on U235, Pu239, Xe135
  - 20 days, constant power
- **MC&D convergence parameters**
  - MC:
    - Number of cycles n = {100, 400} (+30)
    - Number of neutrons N = {800, 3200}
  - Depletion time step dt = {6, 24, 96} hrs



A first MC discrepancy benchmarking

- **Example of result**

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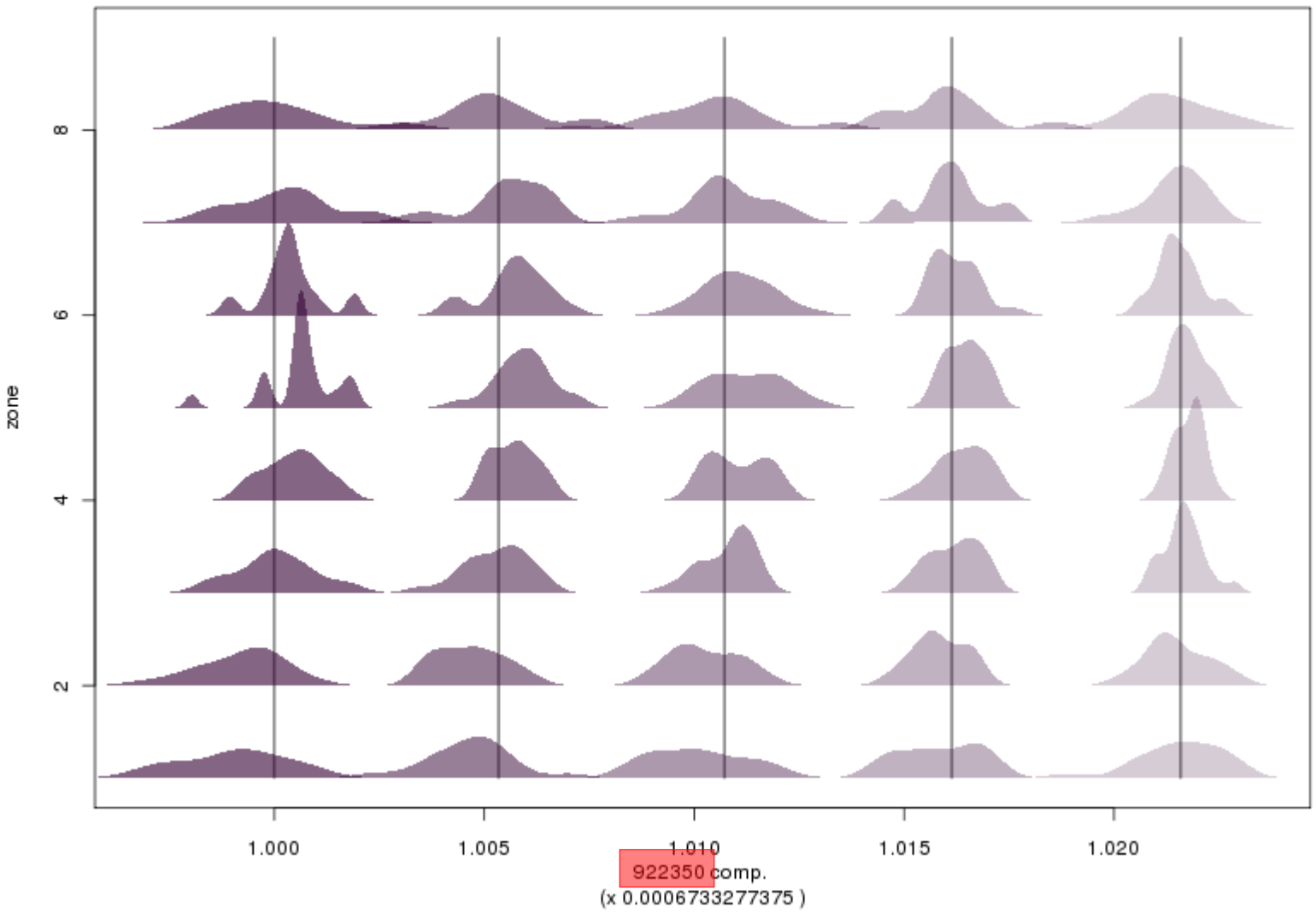
922350 comp.
(x 0.0006733277375)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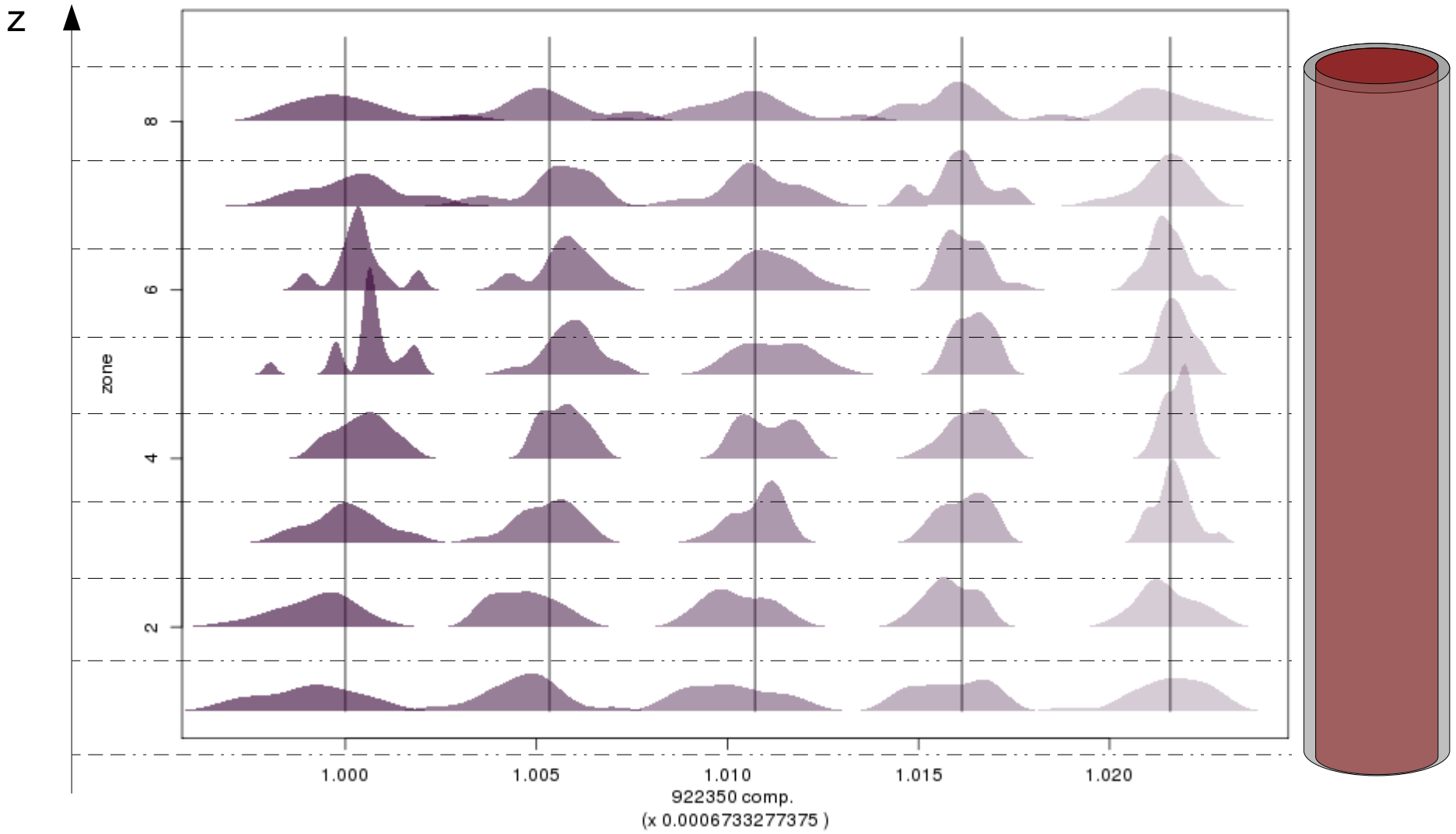
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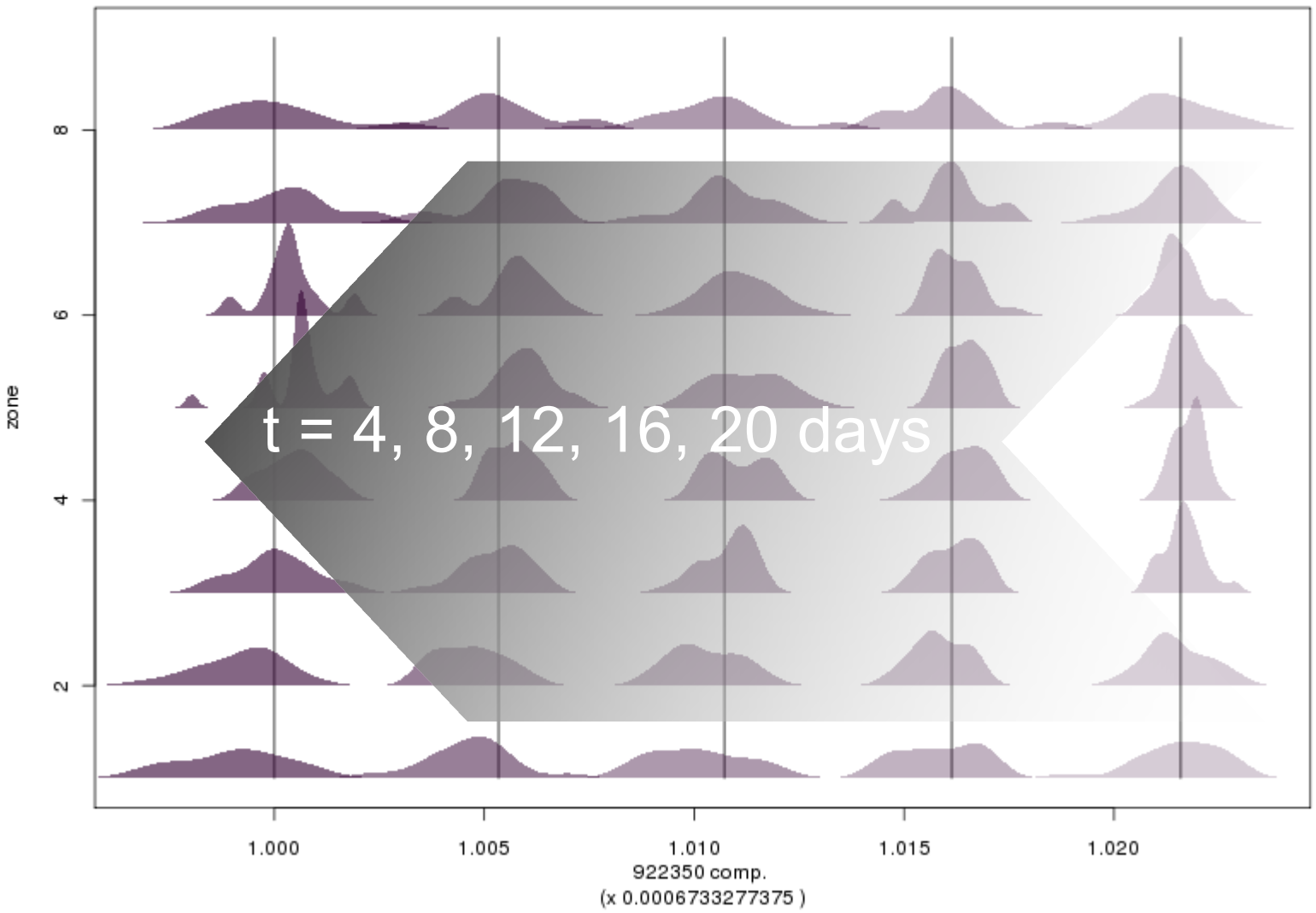
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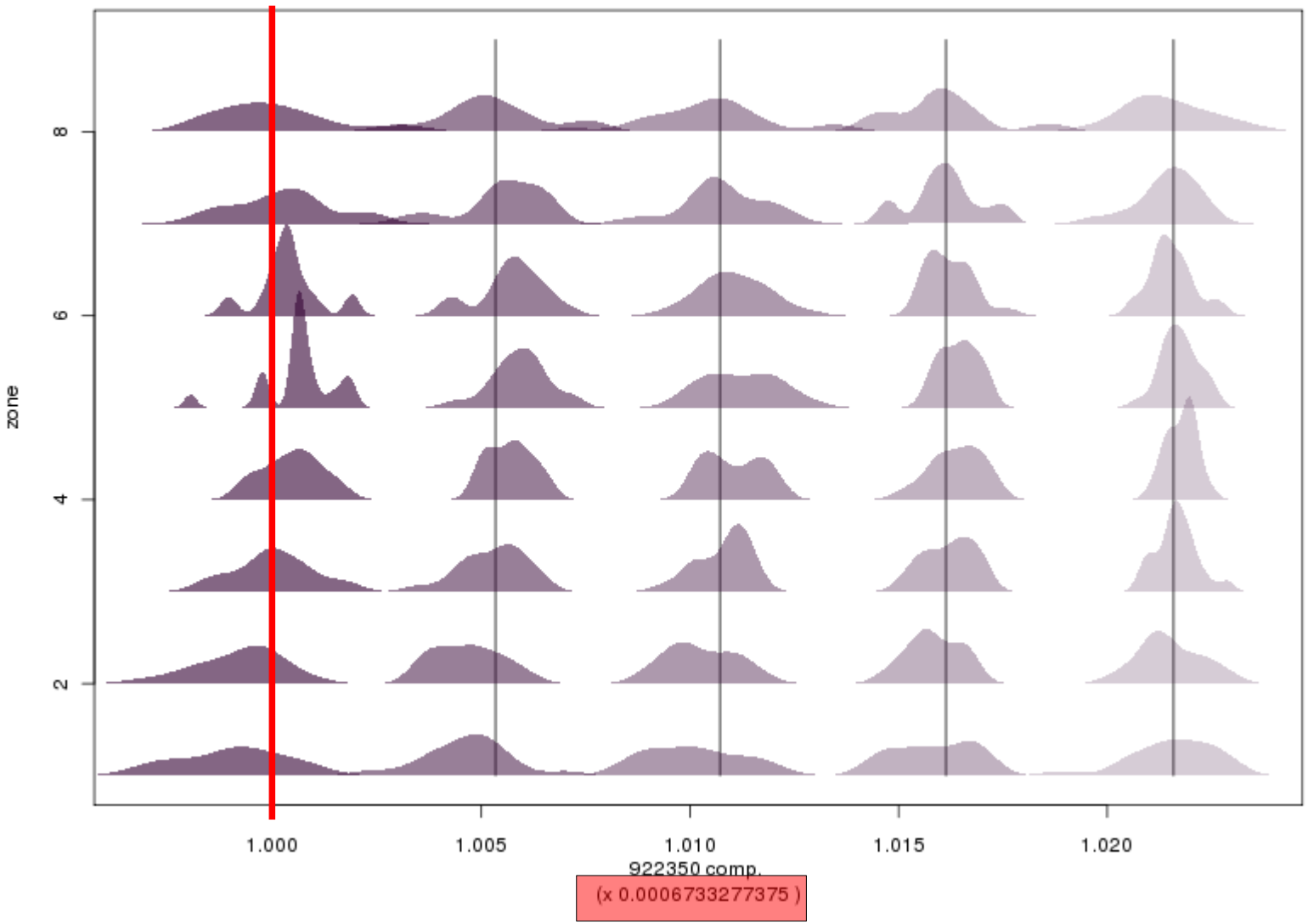
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A first MC discrepancy benchmarking

U235

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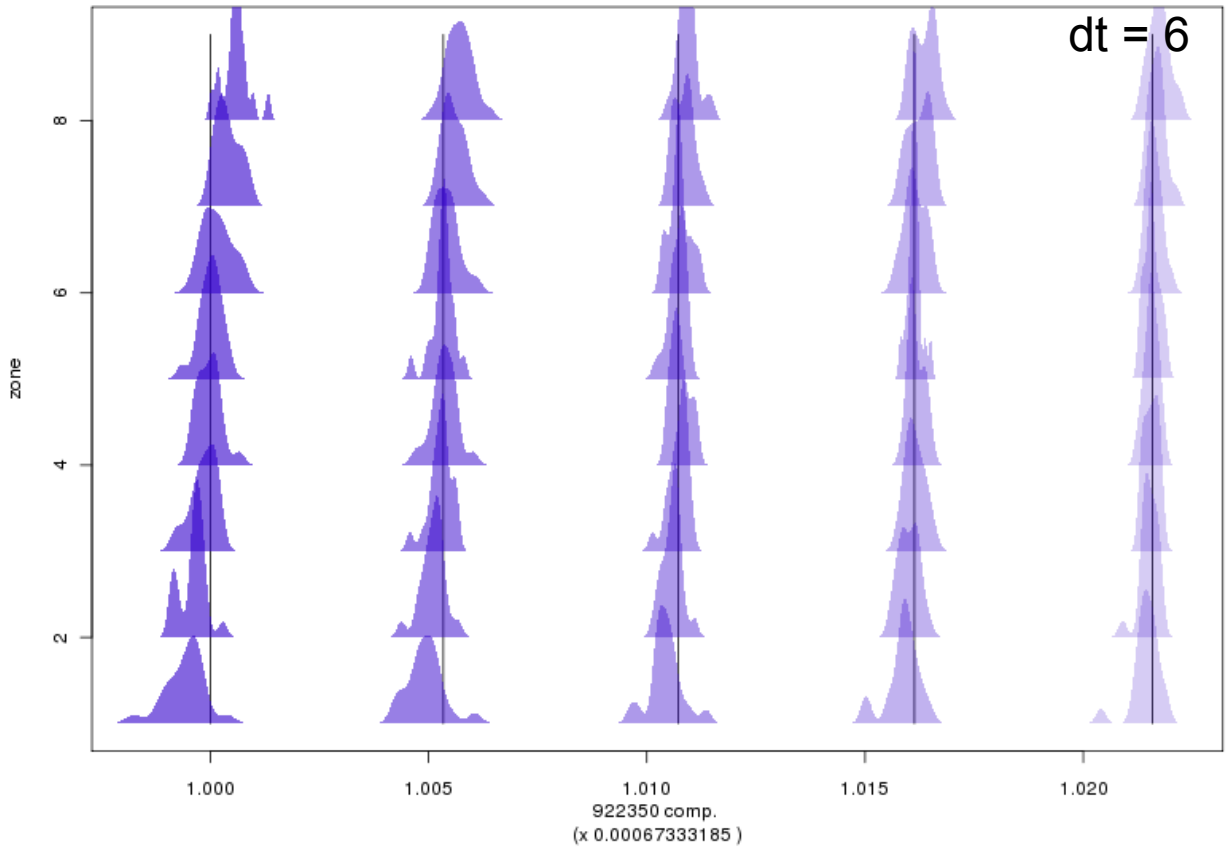

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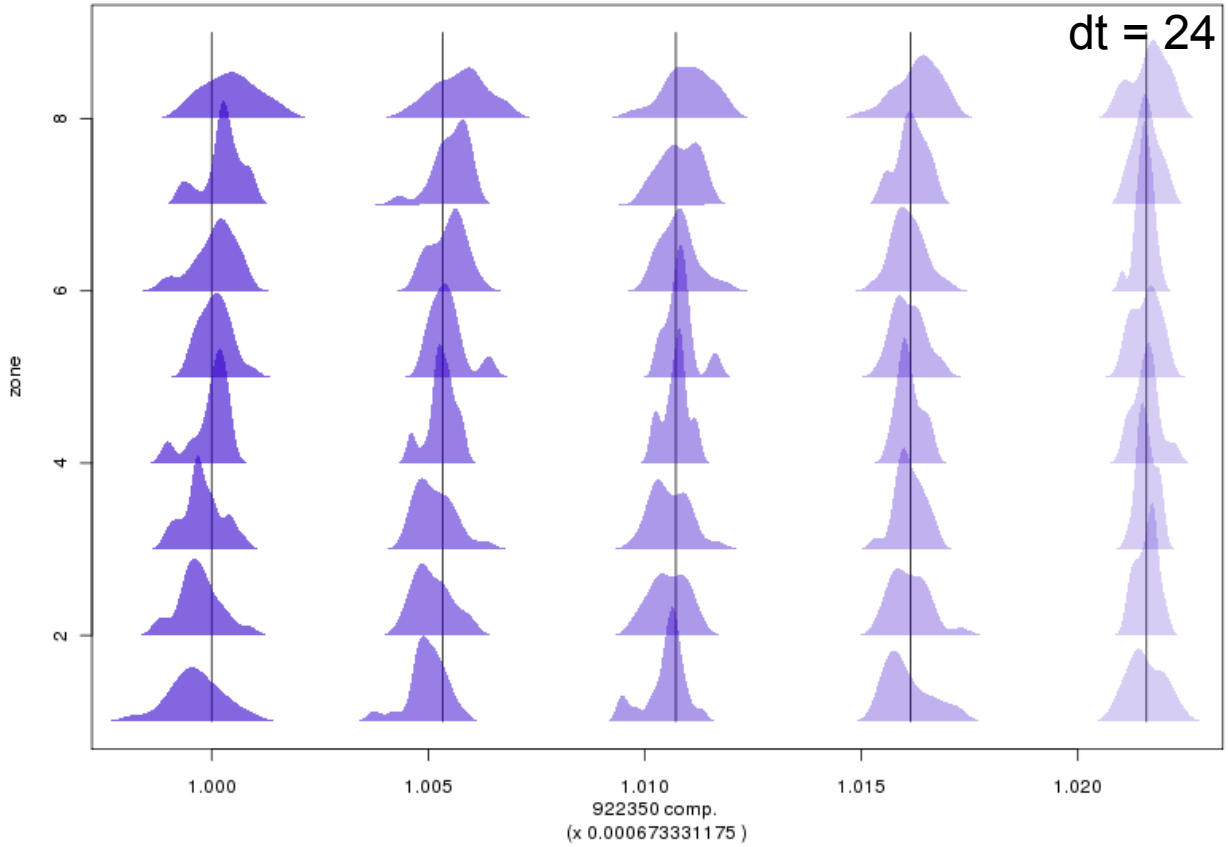

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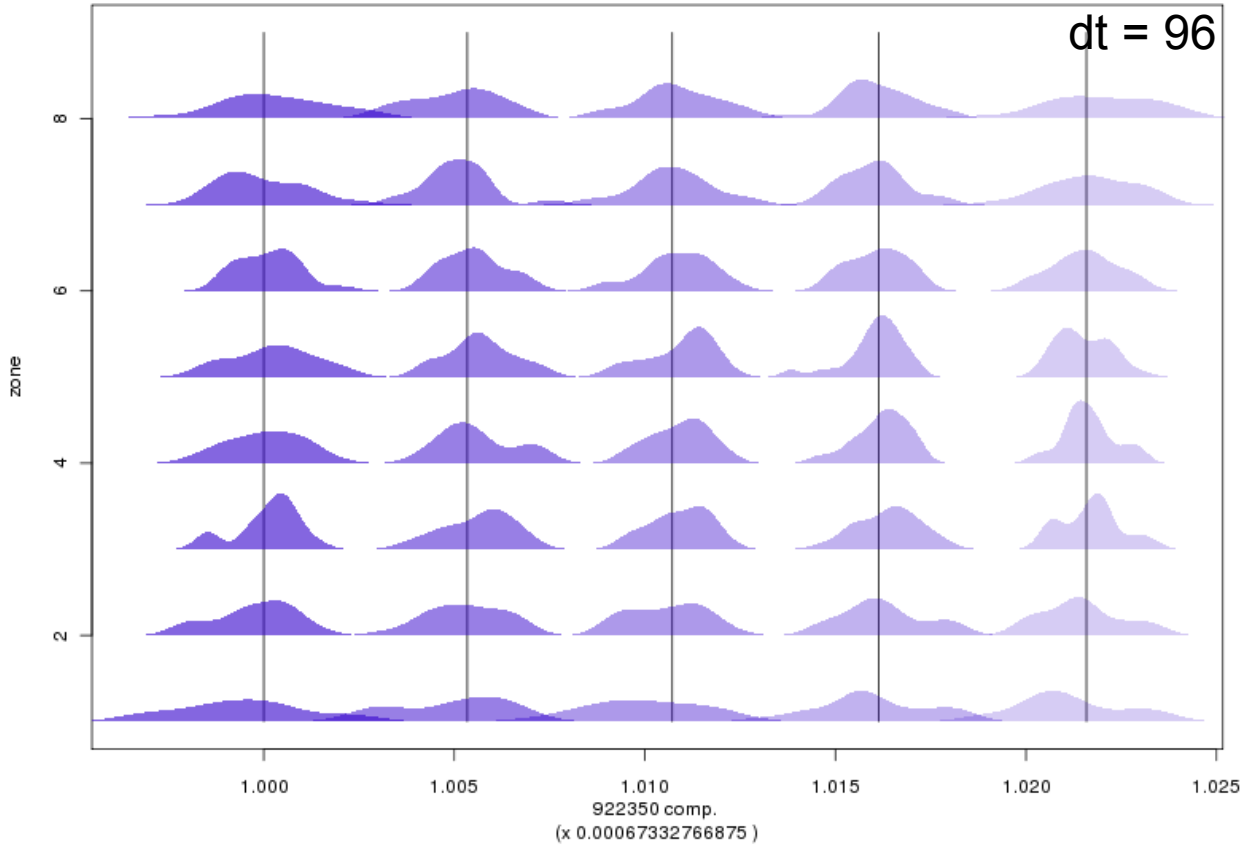

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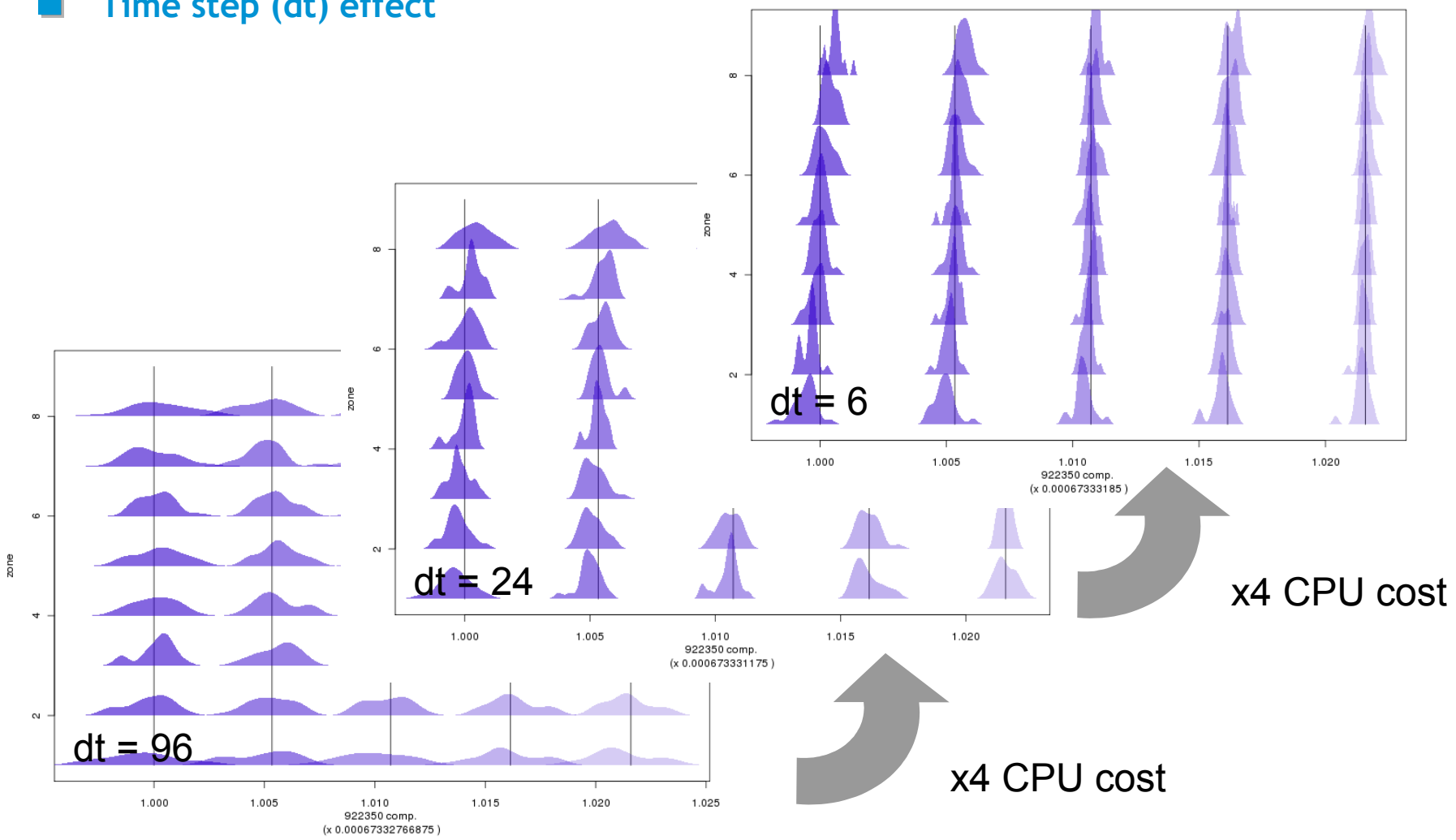

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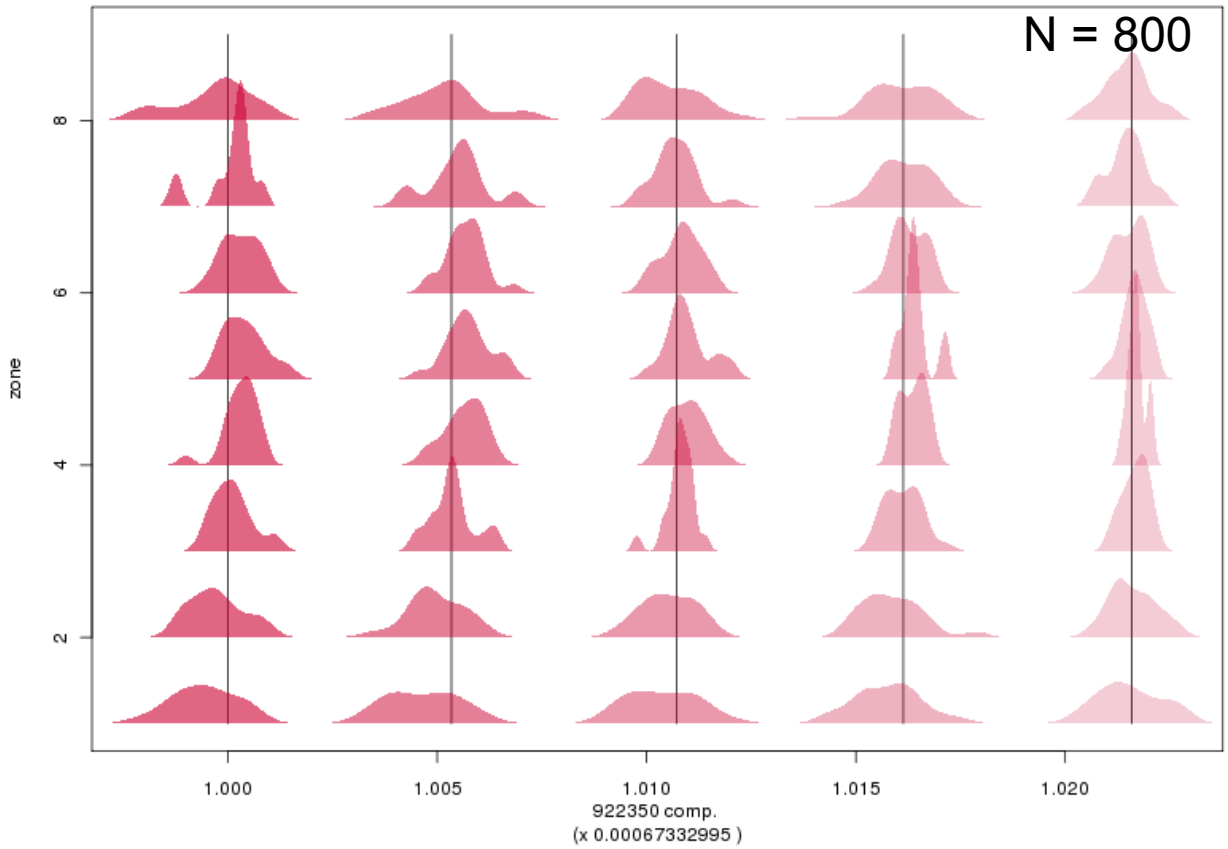

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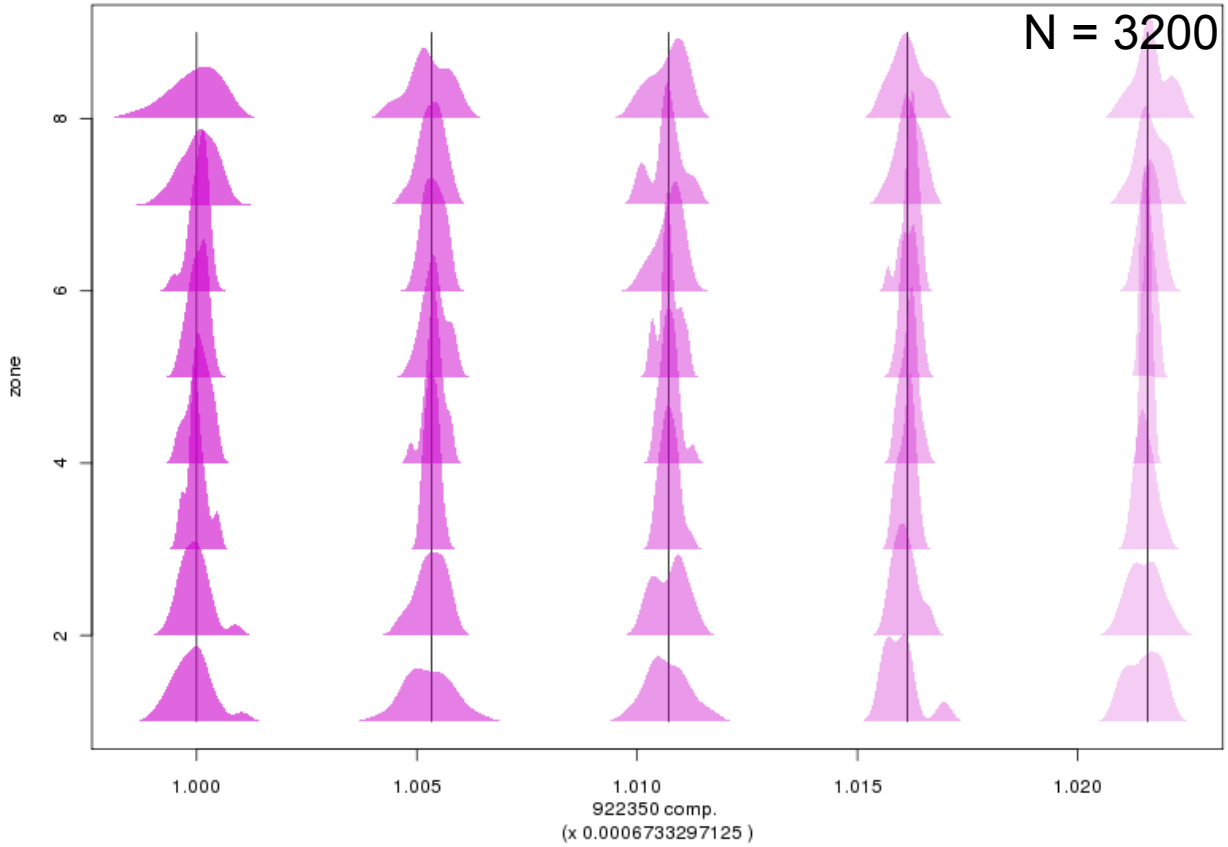

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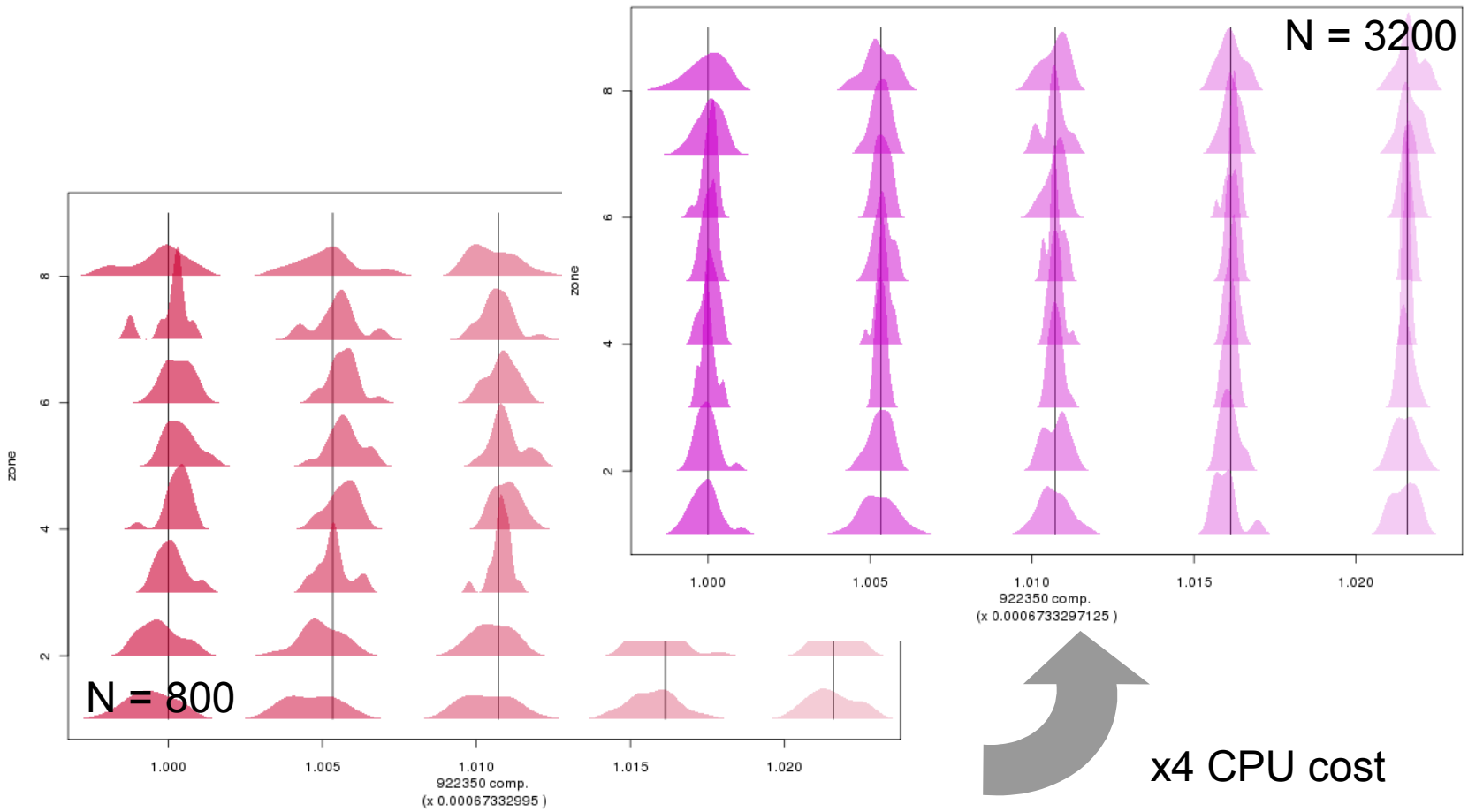

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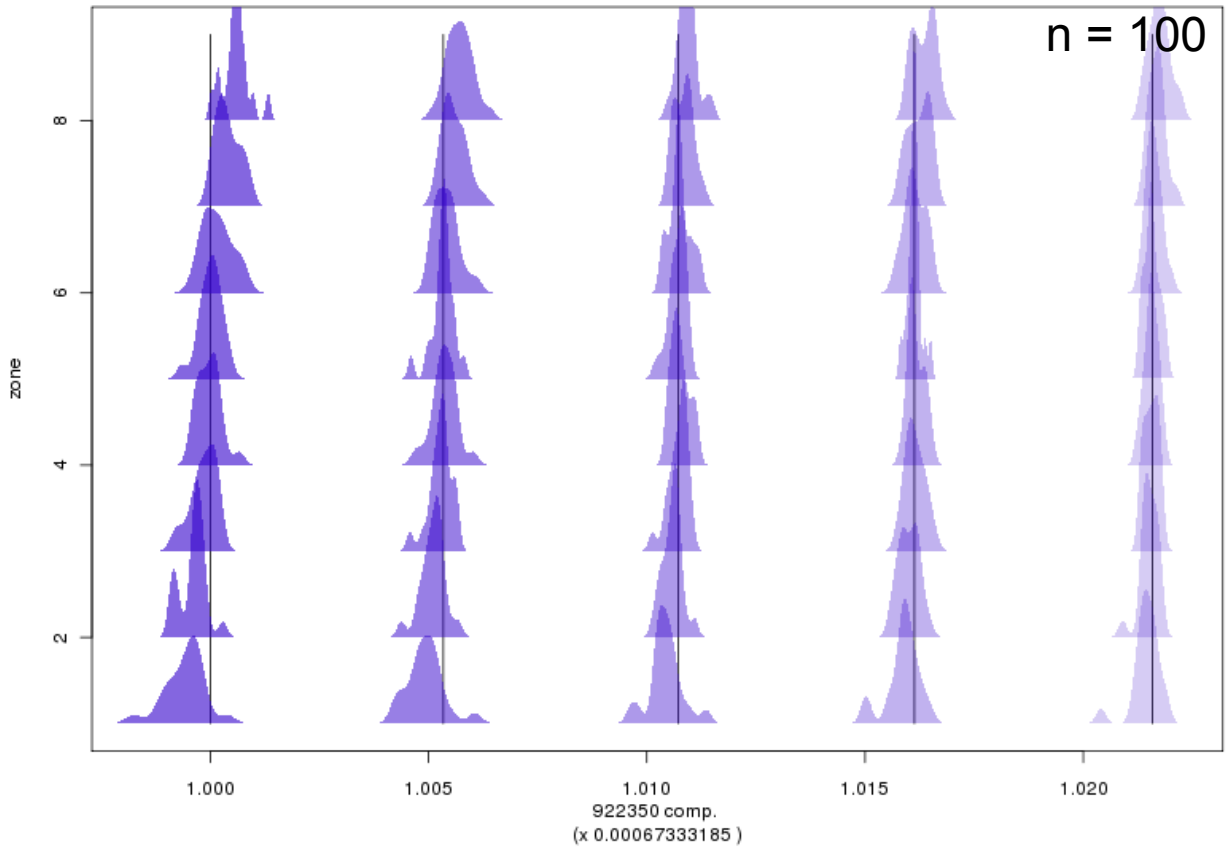

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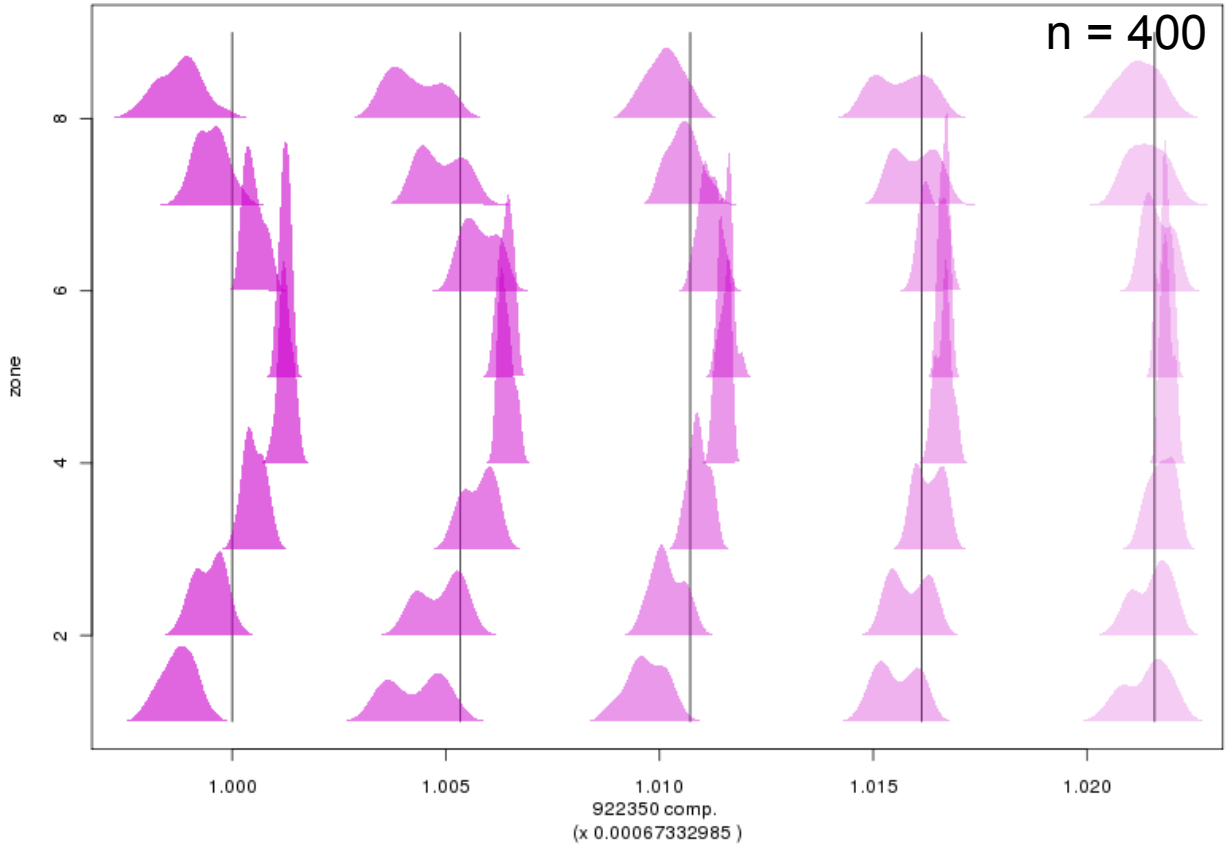

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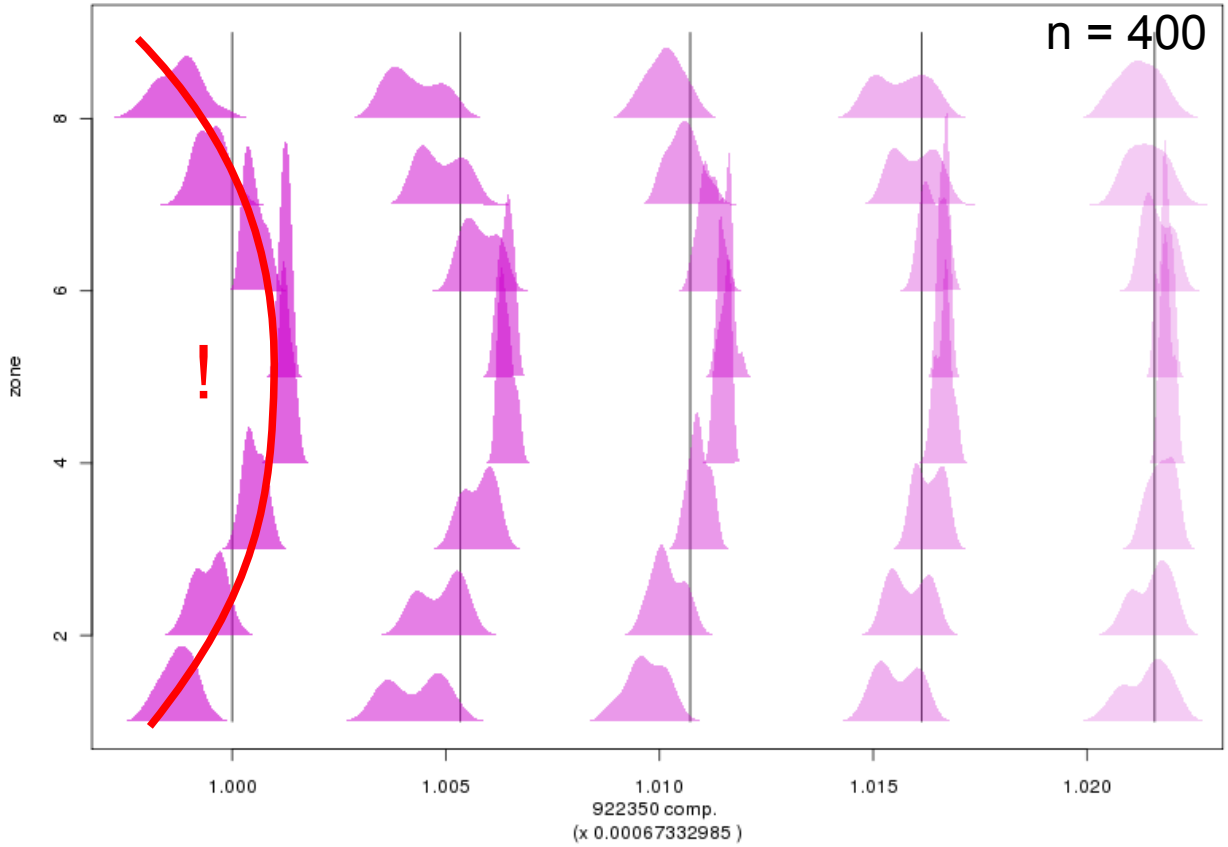

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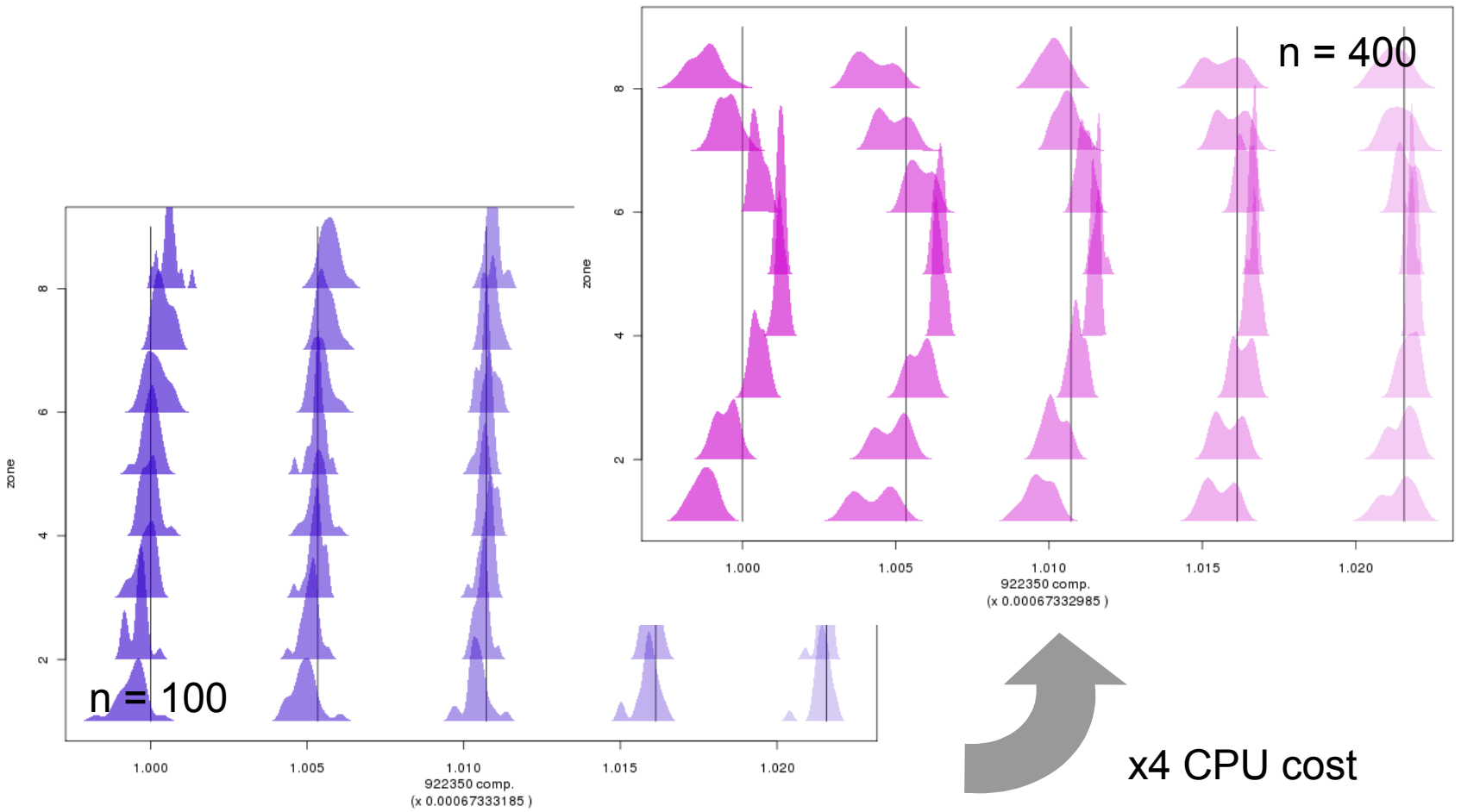

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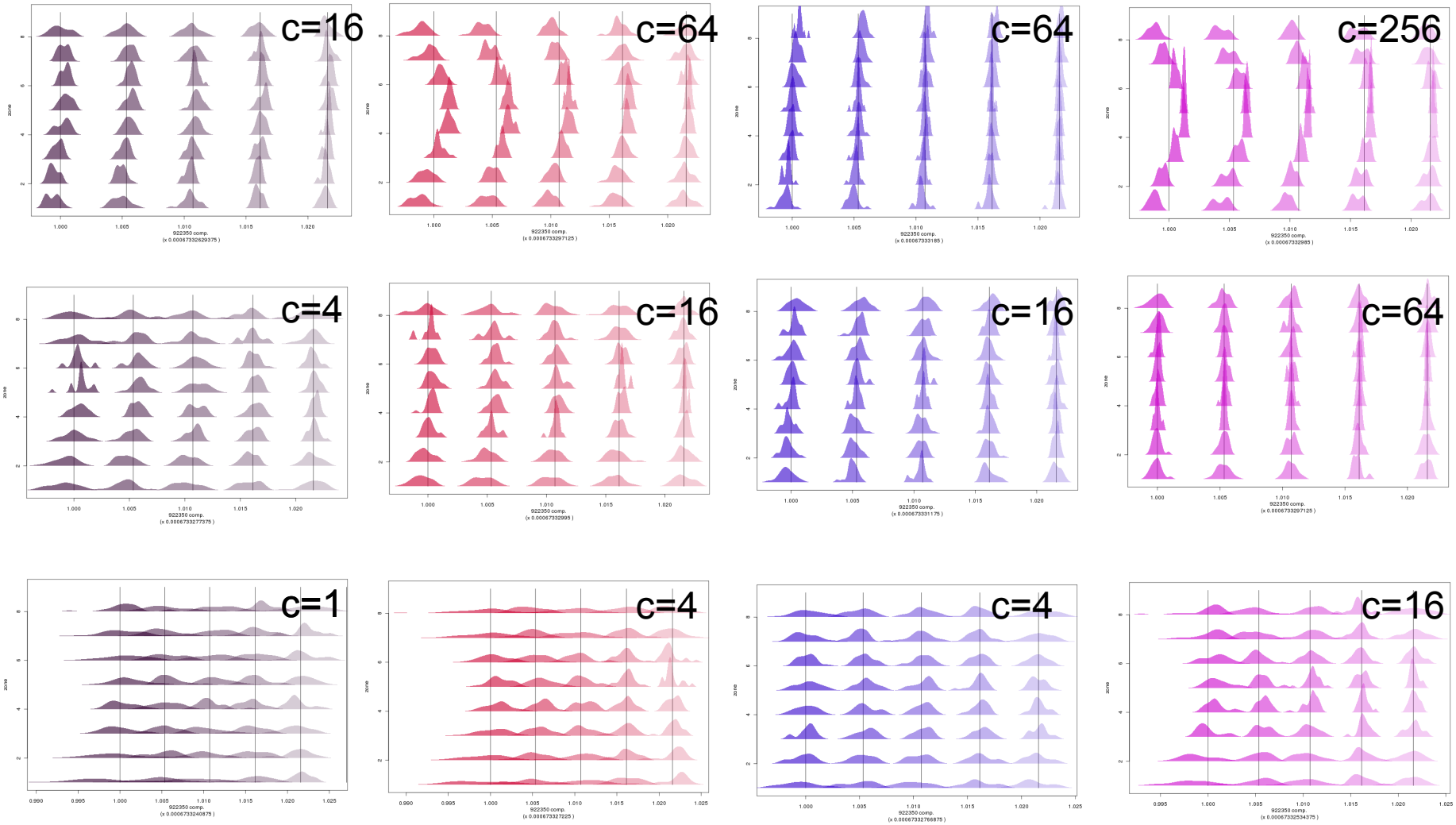

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Pu239

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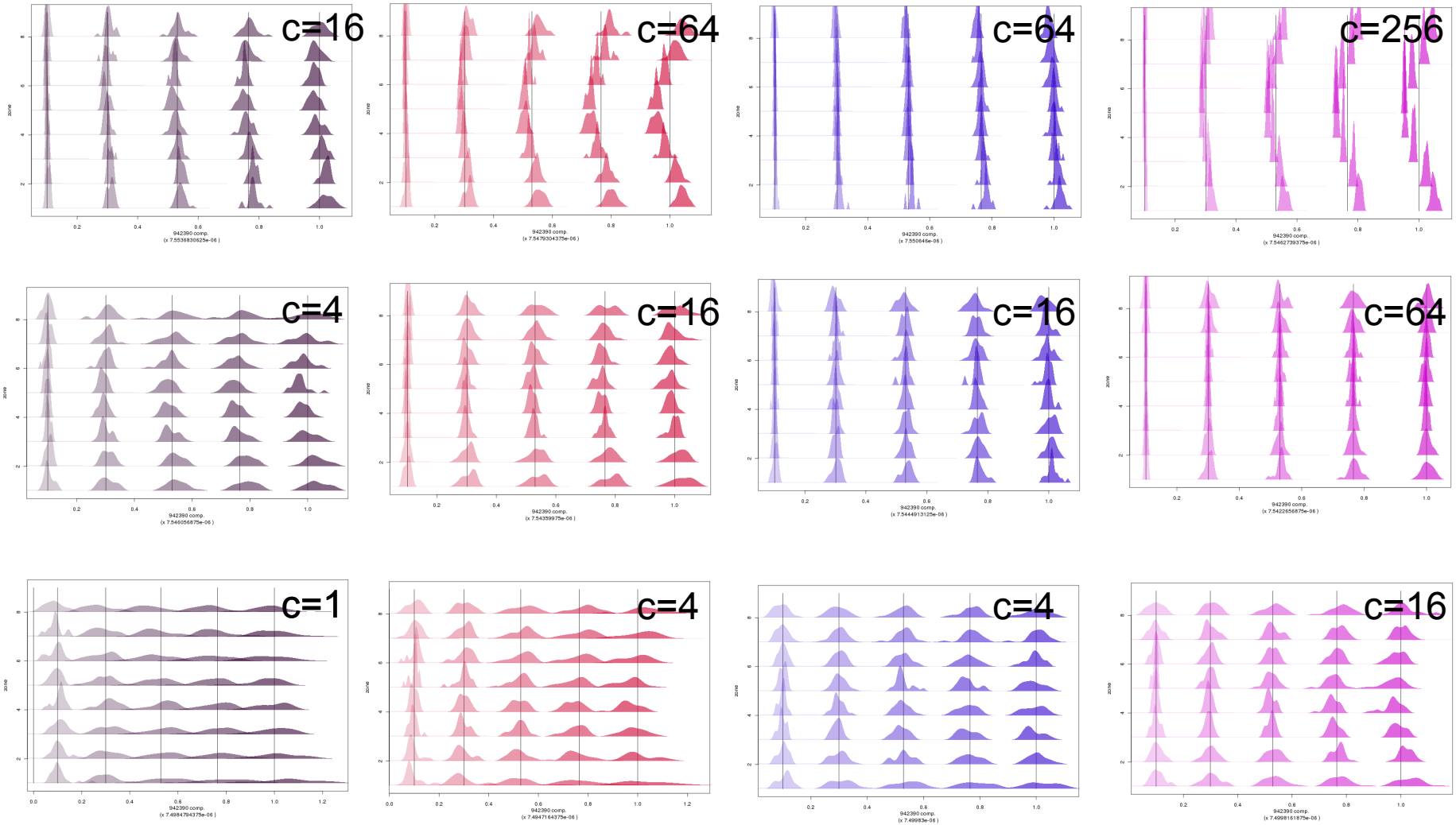

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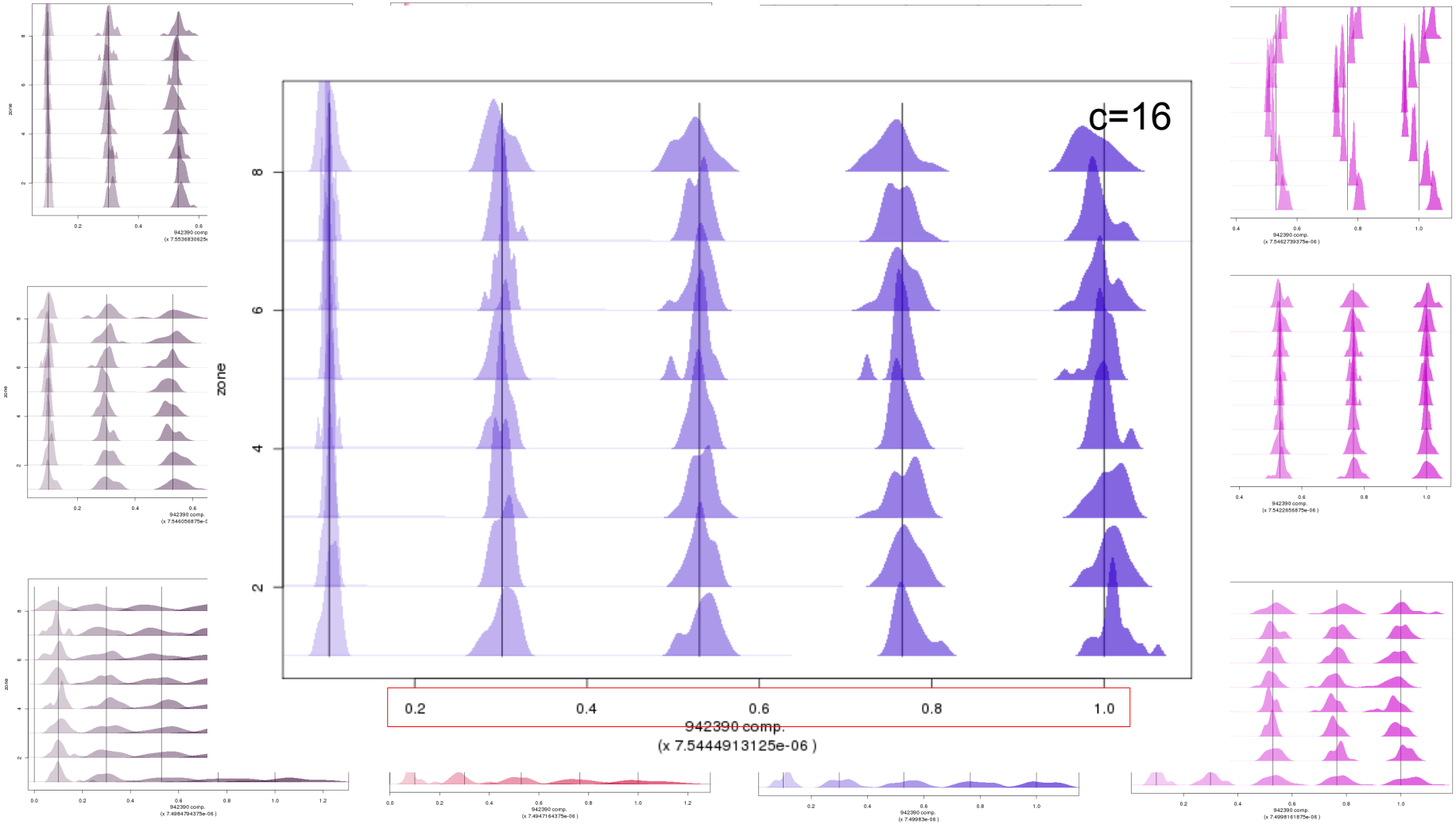

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Xe135

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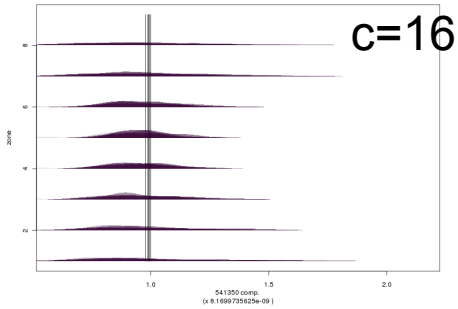
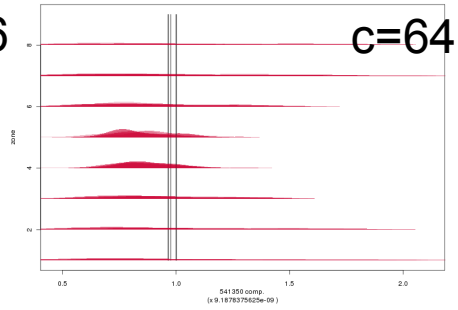
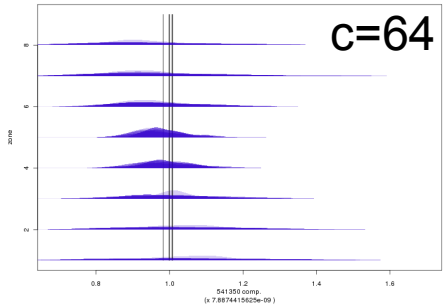
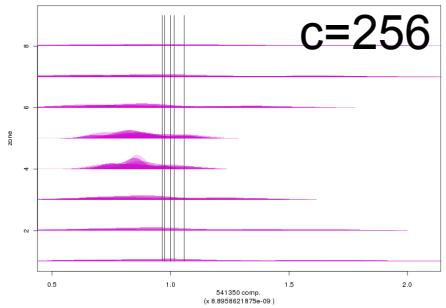
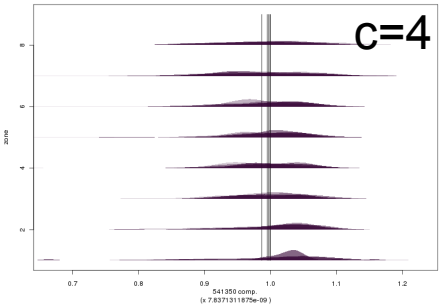
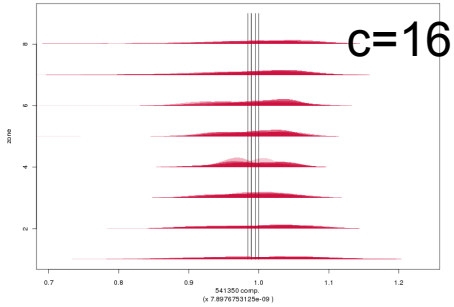


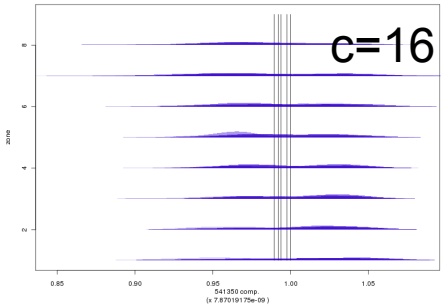


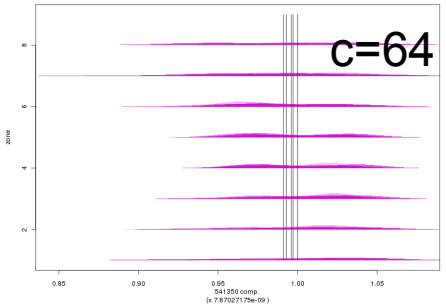


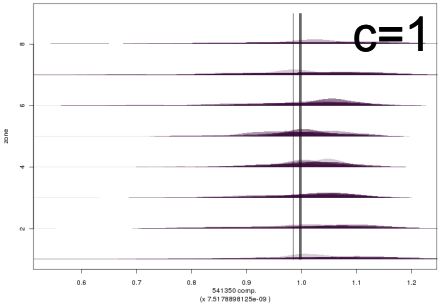


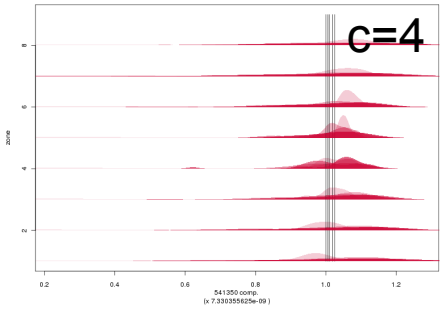


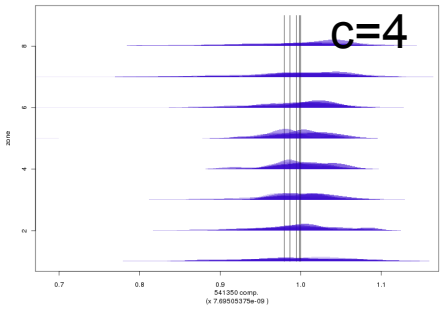


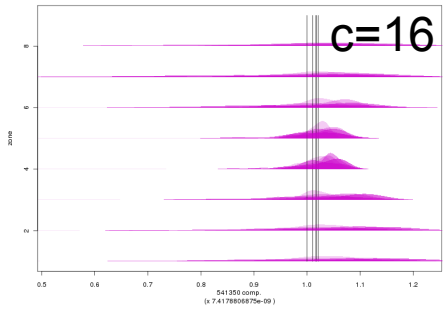




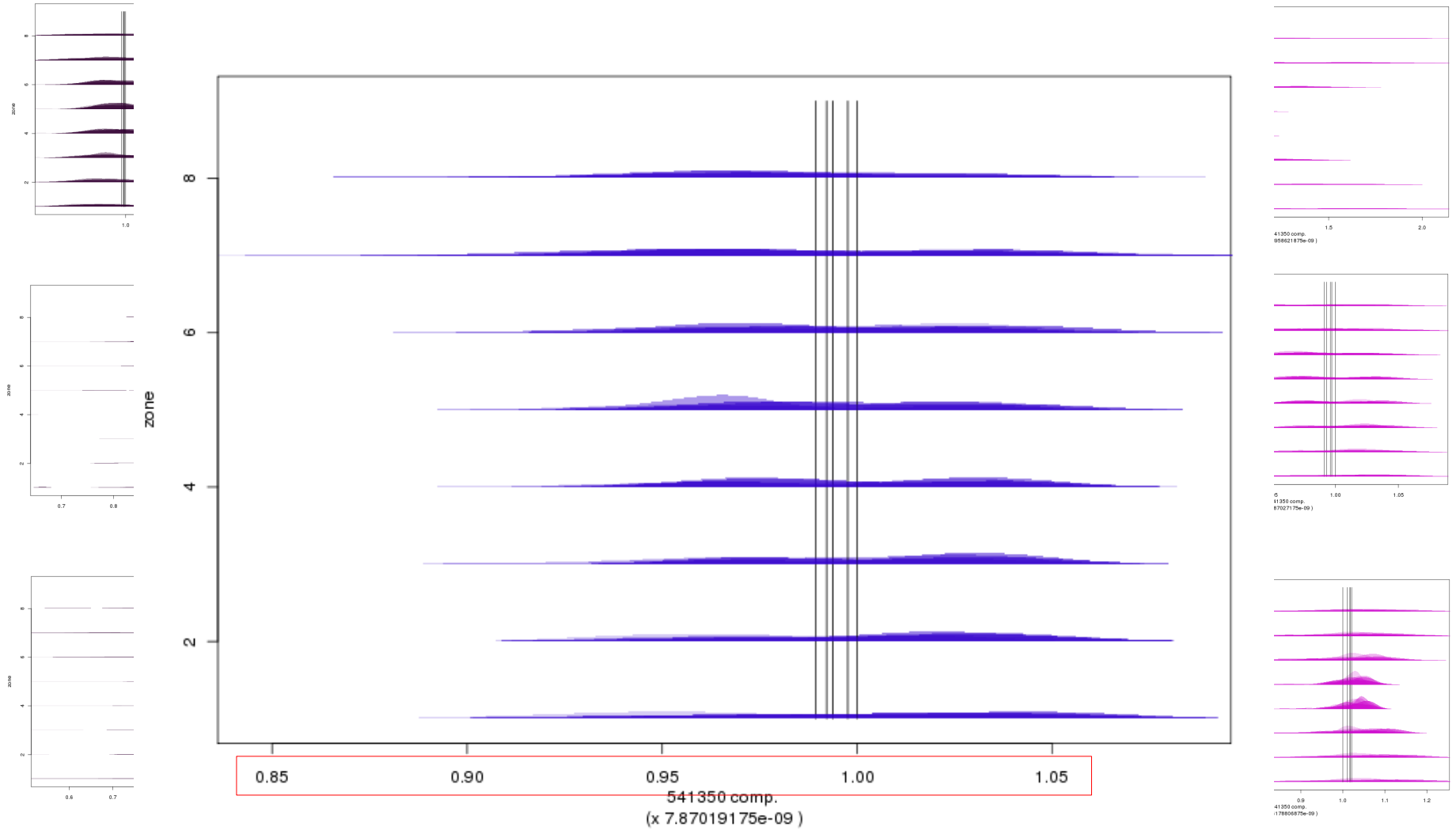








A first MC discrepancy benchmarking



A first MC discrepancy benchmarking

- **MC cycles (n)**
  (combined with Z reflections) seems to lead to
  - Bias of composition expectation
  - Larger uncertainty
- **MC sources (N)**
  - High number of sources limits spreading
  - Z reflection to be studied
- **Depletion time step**
  - Spreading seems to stabilize after some time steps...
- **Output**
  - U235
    small uncertainties (sd ~ 0.3%)
  - Pu239
    significant uncertainties (sd ~ 2%)
  - Xe135
    large uncertainties (sd ~ 5%)

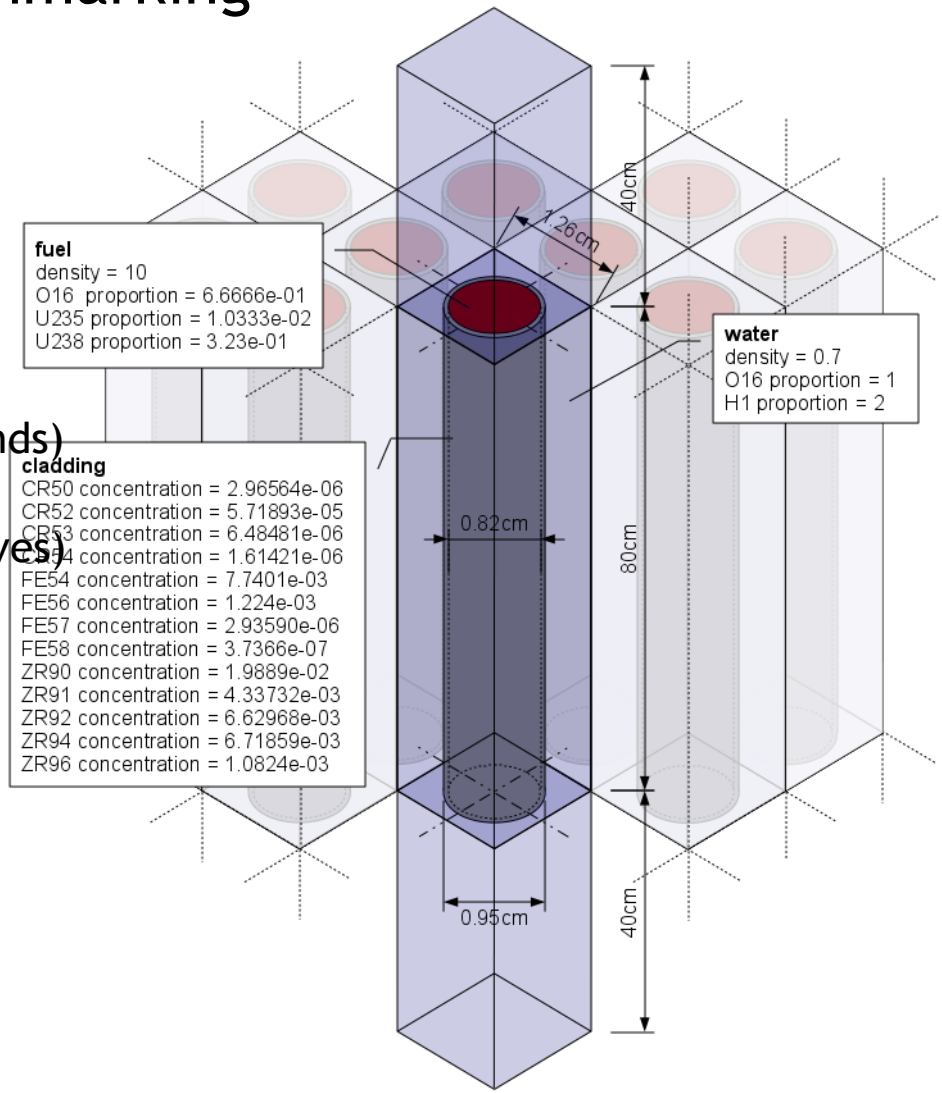
Proposal for extended benchmarking

- **Deeper study of binning**
  related to mean free path of neutrons
- **With, without and Z-cycle reflections**
  (how to set in MCNP ?)
- **Effect of sampling & tracking convergence methods (ex: Wielandt) ?**
- **Quantiles bounding with sample size**
  using two-sided Wilks formula

Proposal for extended benchmarking

- **Proposal benchmark «n zones rod»**
  - n zones rod, n=2^i, i=0..5 (~mfp)
  - with, without, cycle reflections
  - time step = 1.5,6,24,96 h
  - total time >> 20 days
  - 38 random seeds
    (for 90%/90% upper & lower bounds)
  - neutrons=800,3200
  - Batches=100,400,1600 (30 inactives)
  - focus output compositions:
    Z = 92235, 94239, 53135, 54135

  - Variance reduction
    - Sampling
      - Analog
      - Stratified in volumes
      - Superhistory
      - Wielandt (MCNP, MORET, …)
    - Tracking
      - Path weighting (MCNP)
      - …



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  - Manage Monte Carlo convergence parameters
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  - Manage depletion stability
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  - « True » vs « Best estimate » Monte Carlo
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    - Not necessary high CPU cost, thanks to raw CPU parallelization

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- **Well conditioned problem for deterministic calculations**
  may be ill conditioned for Monte Carlo
  … and vice-versa …