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Simple, stable Monte Carlo and depletion

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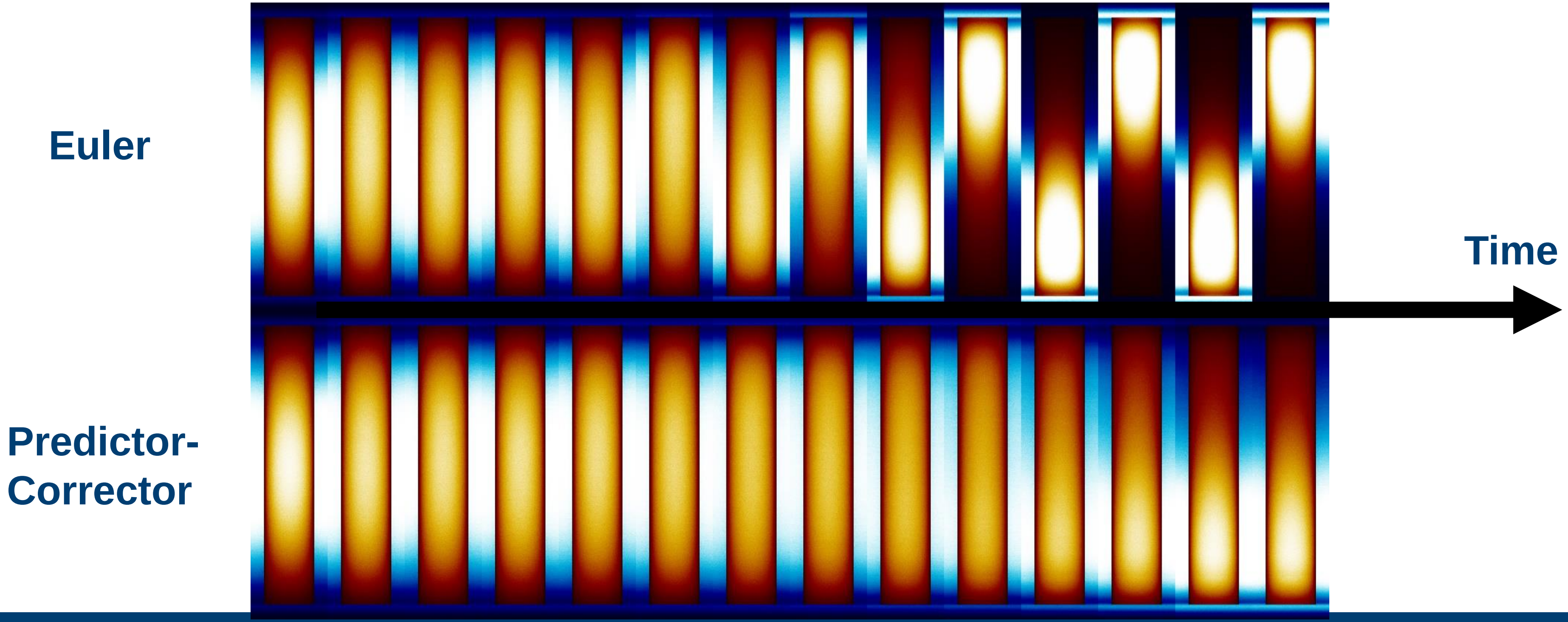
Engineering - Energy, Fluid dynamics and Turbo-machinery

Contents

Monte Carlo/depletion instability

- Standard 3.66m PWR pin, uniform coolant density, reflective radial boundaries, vacuum axial boundaries
- 20 day time-steps at most, up to 180 days of burn-up
- 30,000 particles per cycle, 2,000 active cycles, 200 inactive cycles



Short time-scales

A number of authors have shown confounding behaviour with coupled MC/burn-up on time-scales ~hours

- **Isotalo et al. (2013):** PWR pin, fully reflective boundaries, 15 minute time-steps – oscillations trigger
- **Josey (2017):** same problem, 3hour steps, much larger statistics – oscillations trigger even when using Stochastic Implicit Euler (SIE)
- **Johnson & Kotlyar (2018):** variable coolant density, axial vacuum boundaries <1 day step – all burn-up schemes disagree significantly

Isotalo, A., Leppanen, J., and Dufek, J. (2013). Preventing xenon oscillations in Monte Carlo burnup calculations by enforcing equilibrium xenon distribution. *Annals of Nuclear Energy*, 60:78-85.
Josey, C. (2017). *Development and Analysis of High Order Neutron Transport-Depletion Coupling Algorithms*. PhD thesis, Massachusetts Institute of Technology.
Johnson, A., and Kotlyar, D. (2018). Comparative Study of Monte Carlo Burnup Scheme for Full Core Calculations. *Proc. PHYSOR 2018.*

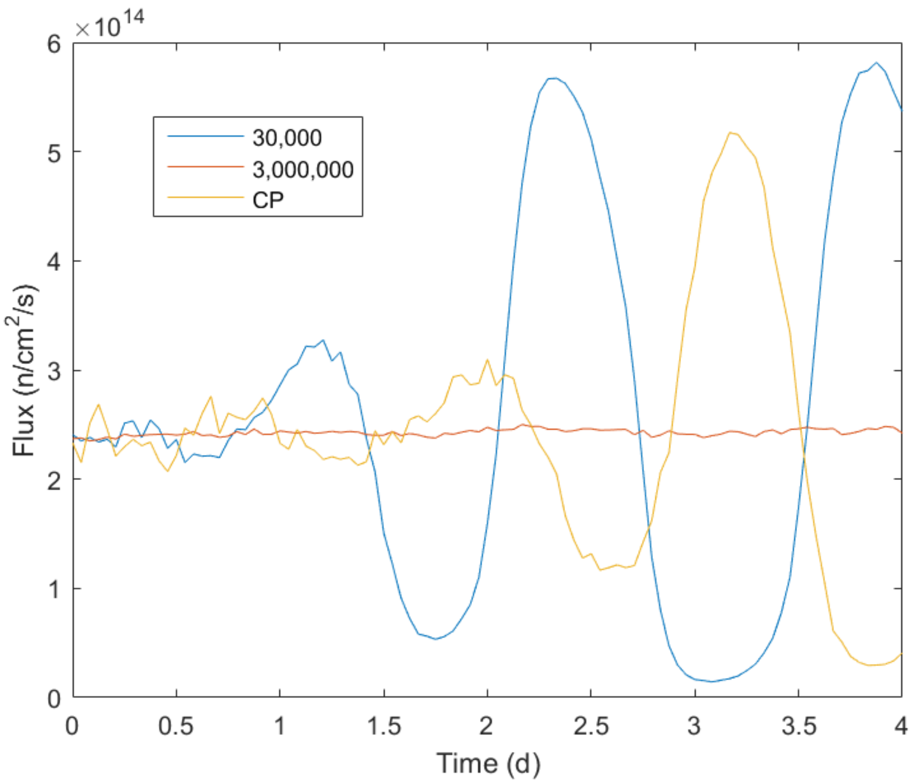
Short time-scales

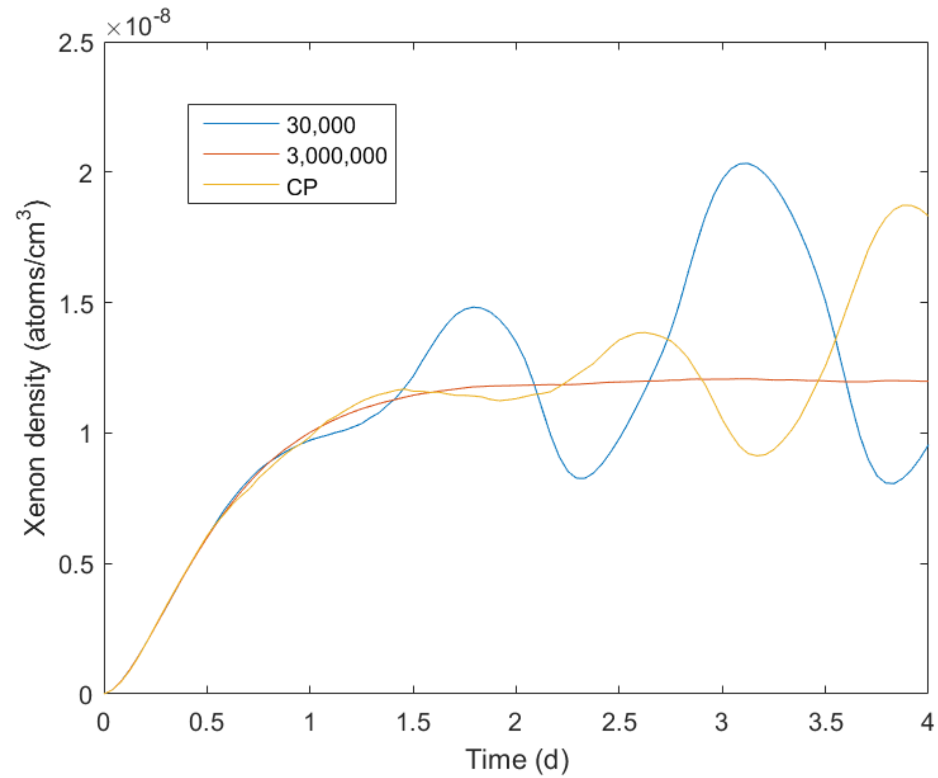
- **Looks to be driven by neutron clustering: few particles/cycle → incorrect transport solution → 'physical' xenon oscillation**
- Take a PWR pin, fully reflective boundaries, 1 hour time-steps,10 burnable regions, explicit Euler scheme
- Three different settings:
  - 'Common practice': 30,000 particles/cycle, 500 active, 100 inactive
  - 30,000 particles/cycle, 5,000 active, 10,000 inactive
  - 3,000,000 particles/cycle, 50 active, 100 inactive

Dumonteil, E., Malvagi, F., Zoia, A., Mazzolo, A., Artusio, D., Dieudonné, C., and De Mulatier, C. (2014). Particle Clustering in Monte Carlo criticality simulations. *Annals of Nuclear Energy*, 63:612-618
Cosgrove, P., Shwageraus, E., Parks, G. (2019). Neutron clustering as a driver of Monte Carlo burn-up instability. *Annals of Nuclear Energy* (in press)

Short time-scales

Look at the flux and xenon density in a single burnable region





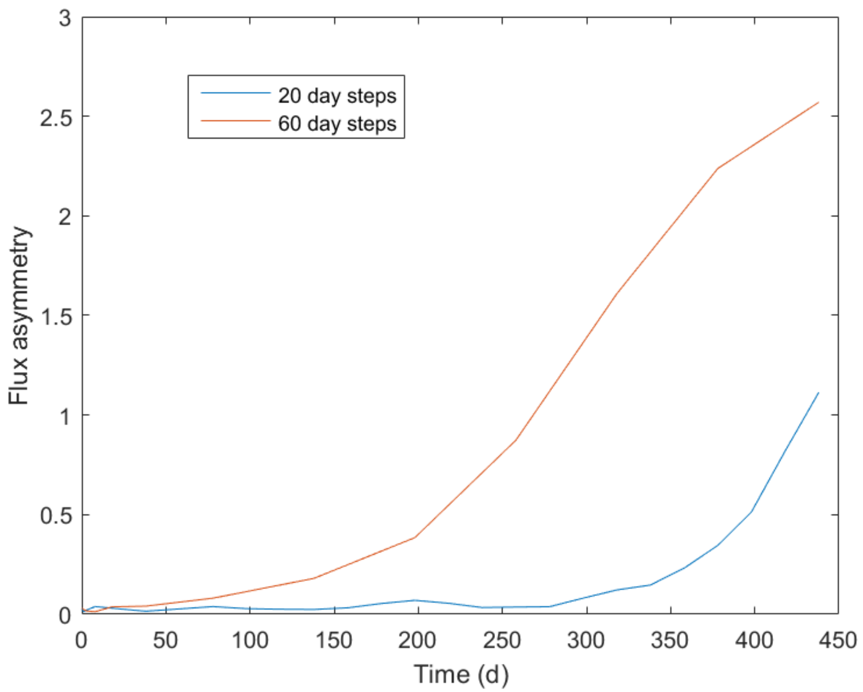
Even explicit Euler appears quite adequate to resolve the correct behaviour for this problem

Longer time-scales

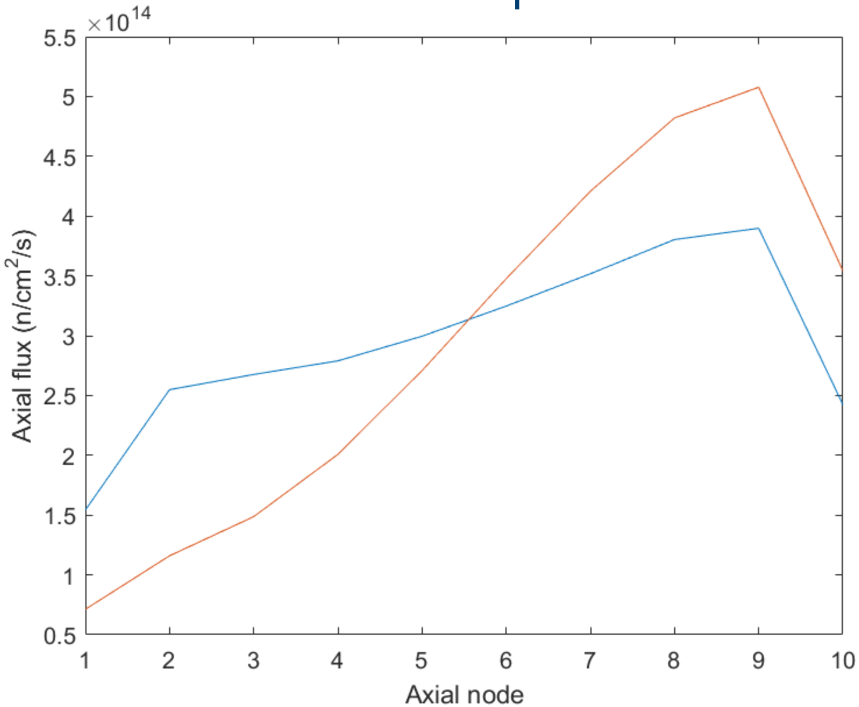
- Accounting for clustering does not seem sufficient to prevent instabilities on longer time-scales
- Take another PWR pin: 3.66m tall, axial vacuum boundaries, uniform coolant density
- Settings: 3,000,000 particles/cycle, 60 active, 10 inactive, accelerated by Serpent’s response matrix solver
- Burn with maximum time-steps of 20 days and 60 days using the standard PC scheme

Longer time-scales

Flux asymmetry with time



Final flux profiles



- ❑ While many particles/cycle improves results, solution eventually becomes non-physical, regardless of step-length
- ❑ Observe classical numerical instability behaviour where larger time-steps lead to an erroneous solution more quickly

Iterating the corrector step

- In classical predictor-corrector methods, there is an explicit (unstable) predictor step and an implicit (stable) corrector step
- The corrector attempts to solve the following equation for the future nuclide density vector:

$$\boldsymbol{N}^{(1)} = \boldsymbol{e}^{\left[A_{BOS}w_{BOS}+A\left(N^{(0)}\right)w_{EOS}\right]\Delta t}\boldsymbol{N}_{\boldsymbol{BOS}} = \boldsymbol{F}\left(\boldsymbol{N}^{(0)}\right)$$

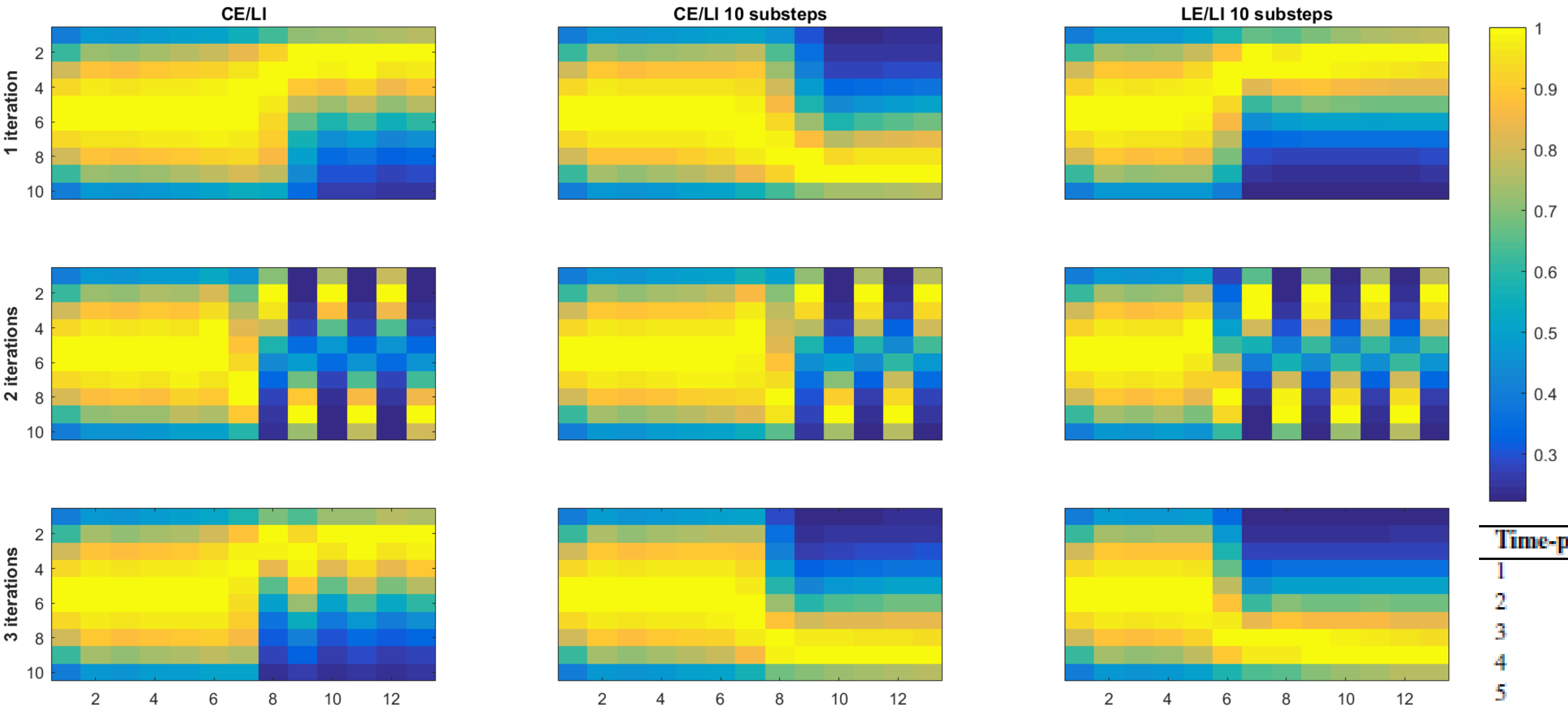
- Instability might be due to $\boldsymbol{N}^{(1)}$ being insufficiently converged – what if we iterate?

$$\boldsymbol{N}^{(k+1)} = \boldsymbol{F}\left(\boldsymbol{N}^{(k)}\right)$$

Iterating the corrector step

- Using a modified version of Serpent, burn-up information is output and depletion is performed by an external MATLAB script
- Allows for iterated corrector (i.e., repeat transport and depletion)
- Done for the PWR pin with axial vacuum boundaries, uniform coolant density
- CE/LI (regular PC), CE/LI with 10 substeps, and LE/LI with 10 substeps are used with 1 to 3 corrector iterations for 60 day max. steps
- 2,000,000 particles/cycle, 80 active, 10 inactive, response matrix acceleration

Iterating the corrector step



Time-point	Time (d)
1	0
2	1
3	3
4	8
5	18
6	38
7	78
8	138
9	198
10	258
11	318
12	378
13	438

- ❑ Iteration does not improve things – either the corrector step is itself unstable (for the given time-step) or it converges extremely slowly
- ❑ Perhaps unsurprisingly, the LE/LI scheme appears slightly more unstable due to the LE step

Relaxing the corrector step

- Relaxation can help stabilise the iterated fixed-point iteration:

$$\boldsymbol{N}^{(k+1)} = \alpha F\left(\boldsymbol{N}^{(k)}\right) + (1-\alpha)\boldsymbol{N}^{(k)}$$

- This is what stochastic-implicit methods do, but with an iteration-dependent relaxation:

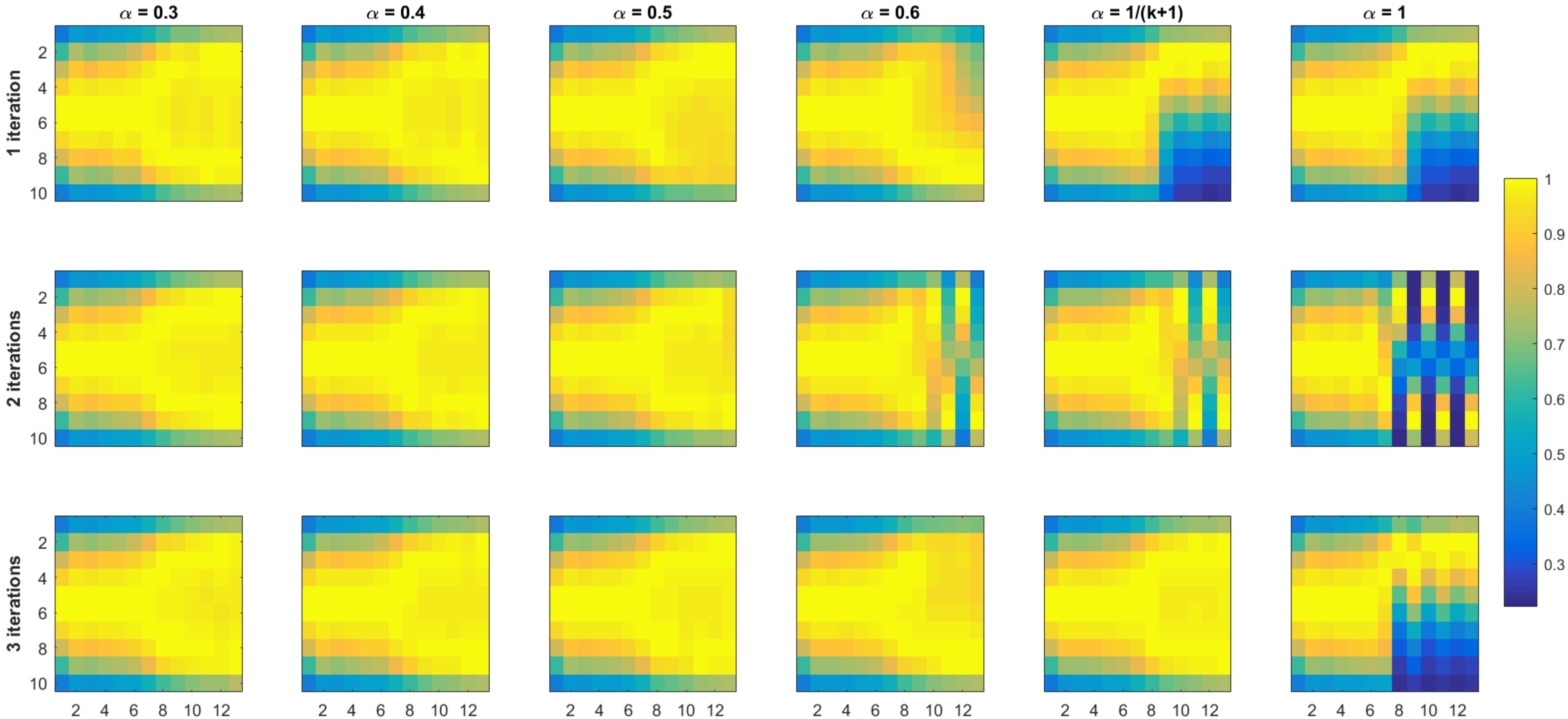
$$\alpha_k = \frac{1}{k+1}$$

- However, SI-methods:
  - Require >10 iterations for long time-steps
  - Equivalent to averaging over iterations – updates become marginal
  - May not be optimal when accounting for clustering

Relaxing the corrector step

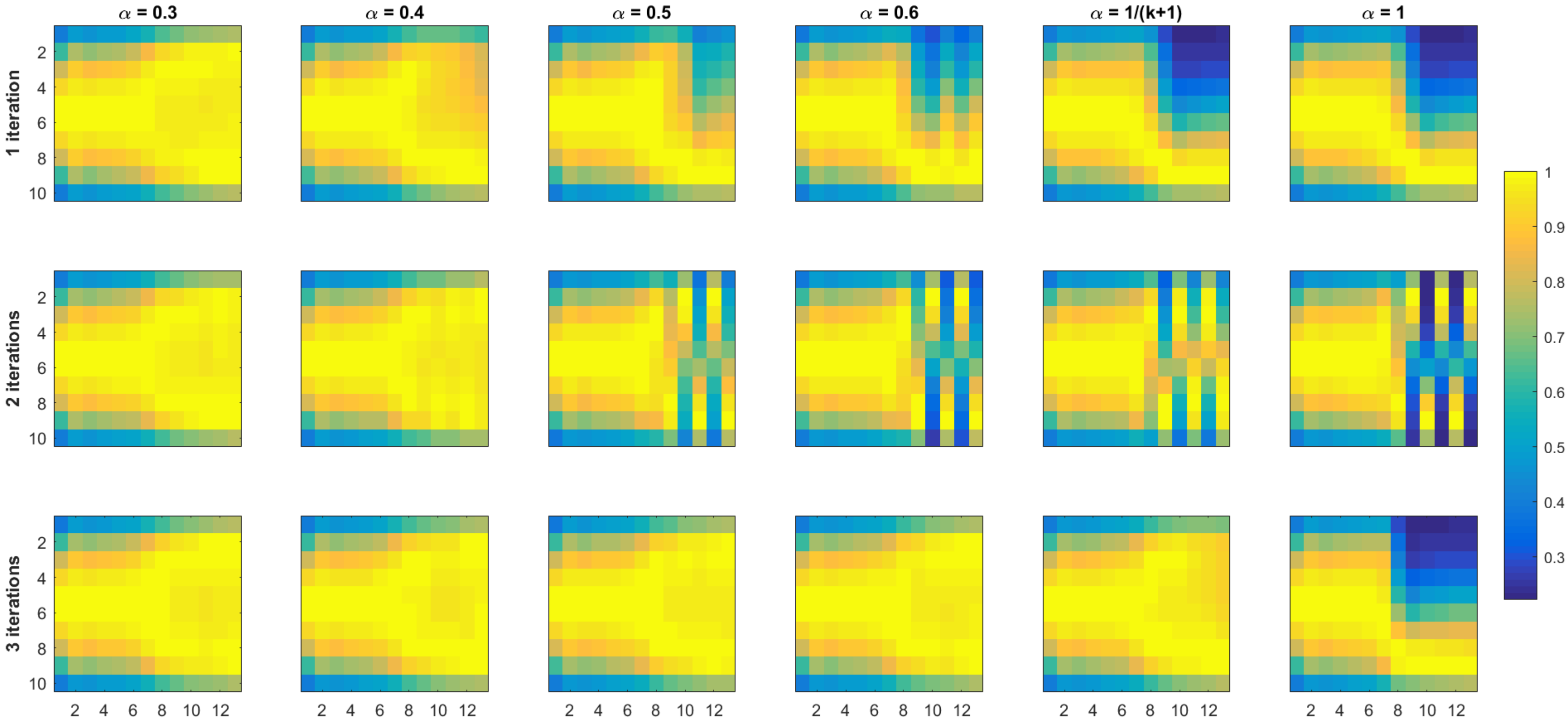
- Consider the same problems as before but varying the relaxation factor from 0.3 to 0.6 and including the SI relaxation
- Use each scheme: CE/LI, CE/LI with 10 substeps, and LE/LI with 10 substeps
- Repeat for 1 to 3 corrector iterations

Relaxing the corrector step – CE/LI with no substeps



Quite mild relaxation, even without iteration, is adequate – however, too aggressive a relaxation may damage accuracy (over-reliance on predictor)

Relaxing the corrector step – CE/LI with 10 substeps



Marginally more unstable than CE/LI without substeps, although 3 iterations with relaxation all appear (mostly) stable

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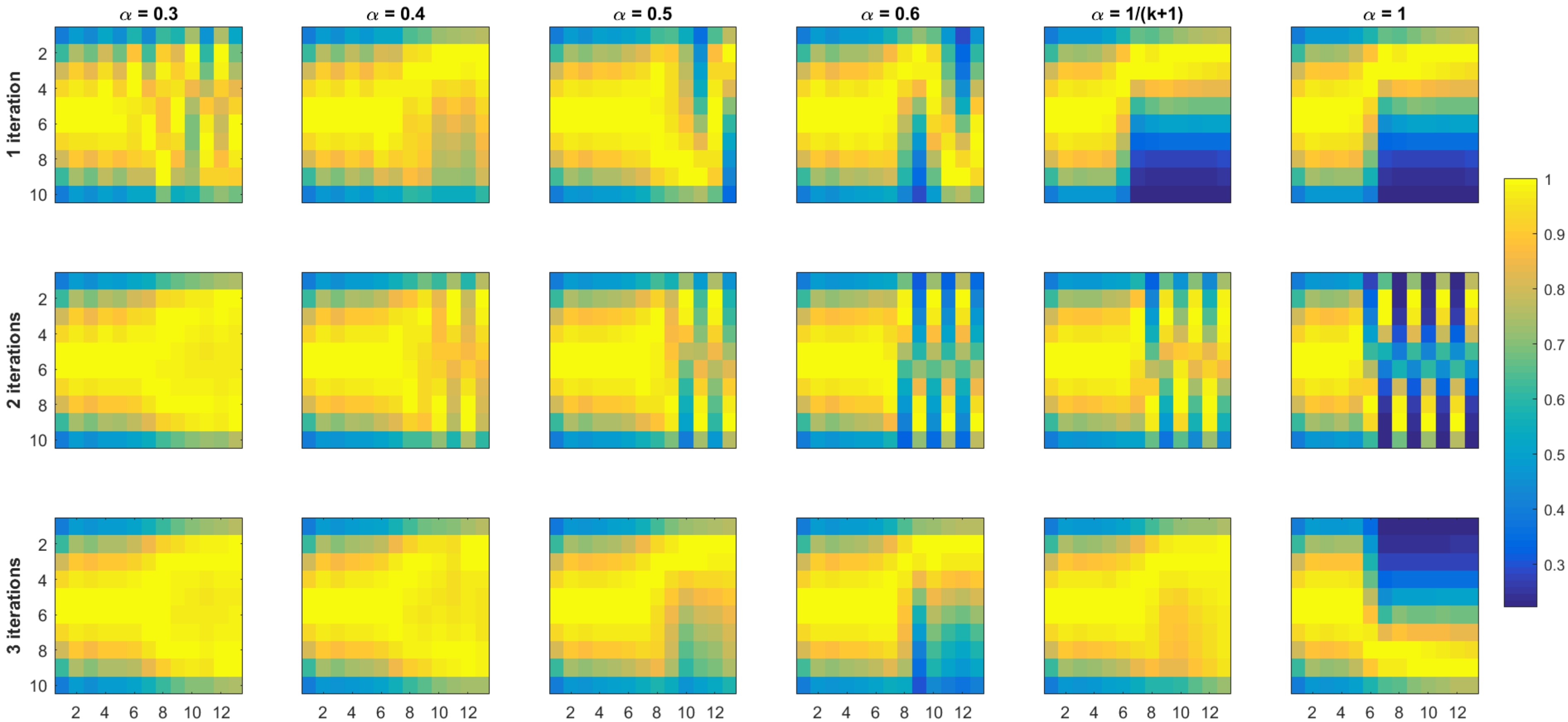
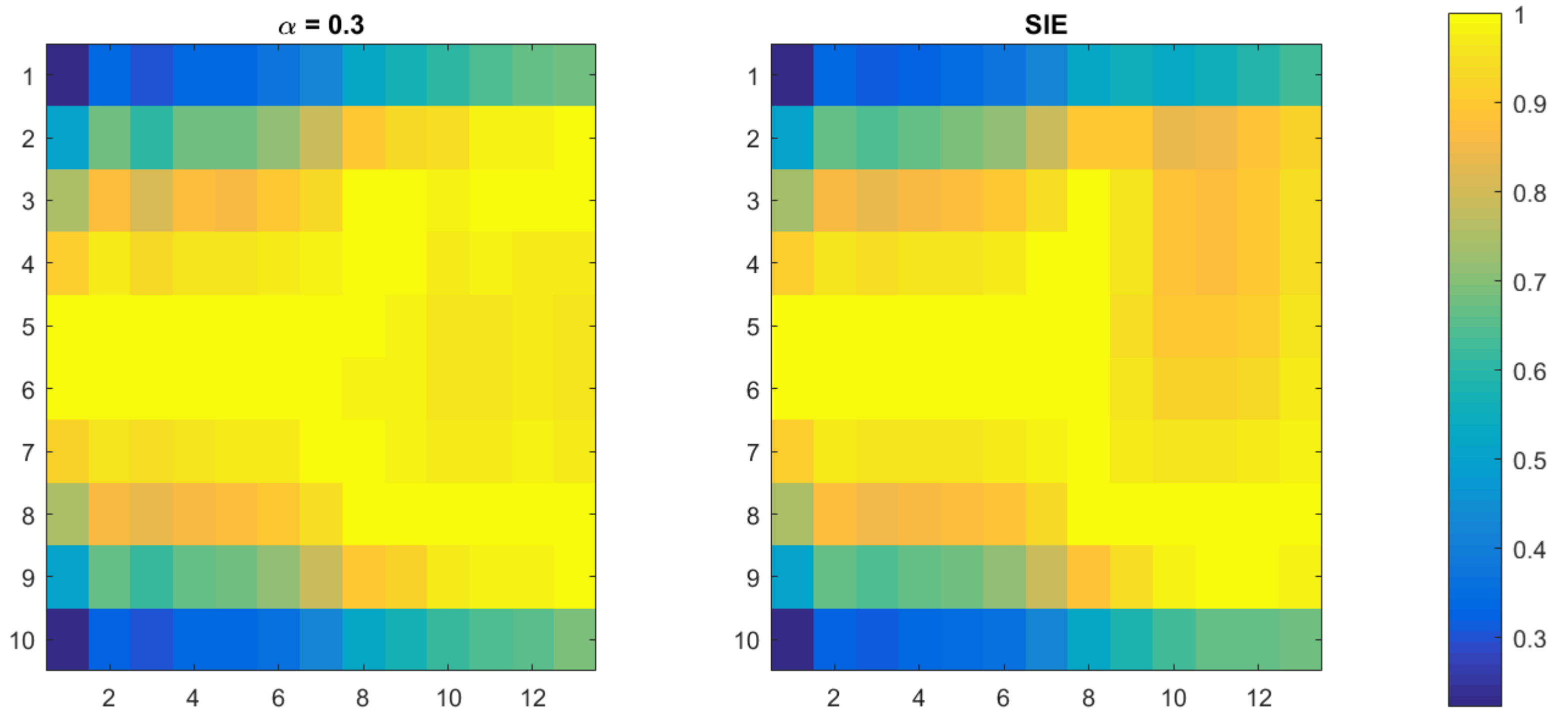
Relaxing the corrector step – LE/LI with 10 substeps



Addition of LE impacts stability greatly – appears to require 3 corrector iterations with substantial relaxation

Relaxing the corrector step – LE/LI with 10 substeps

- How about splitting the stats over 3 corrector iterations?
- Compare 3,000,000/80/10 (accel.) with 3 correctors where the active cycles are split, using SIE and a 0.3 relaxation



Conclusions

- Short time-scale instabilities appear to be primarily due to clustering-contaminated transport solutions
- Longer time-scale instabilities can be more akin to classical numerical instability
- The corrector step is ineffective at locating the fixed-point for time-steps on the order of 20+ days
- Relaxing the corrector step with a fixed relaxation factor can be effective in stabilising the problem – a fixed relaxation is often be more efficient than an SI relaxation schedule

Thanks for listening!

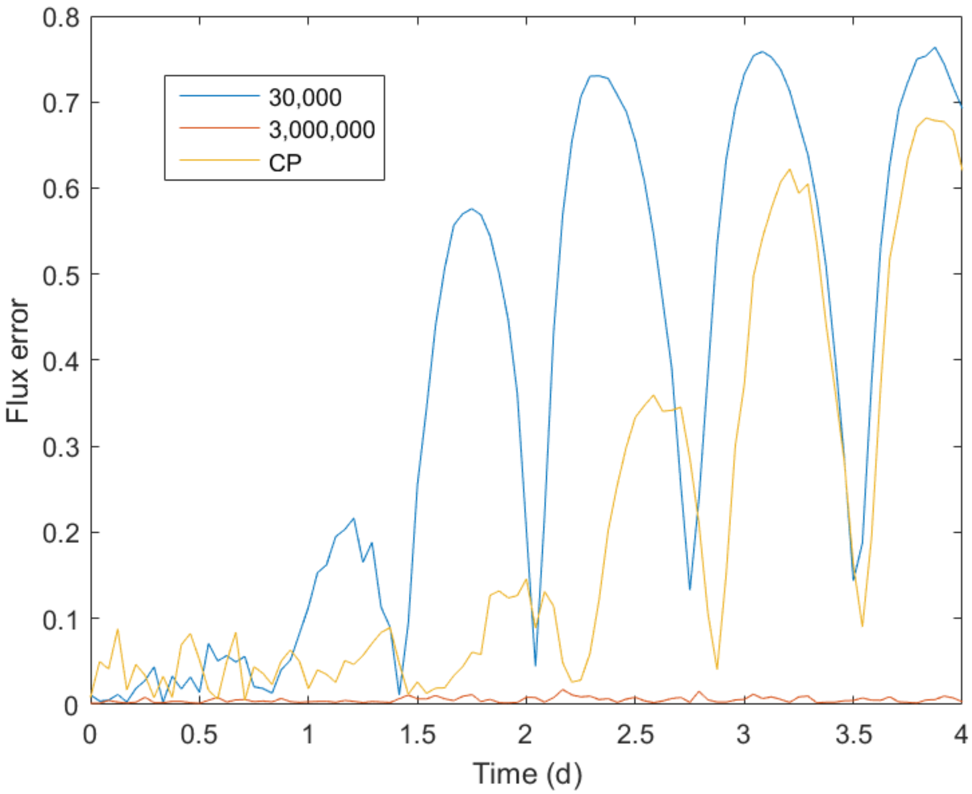
Back-up

Back-up – flux error for short-time burn-up

- Flux error in the reflected pin with a short burn-up

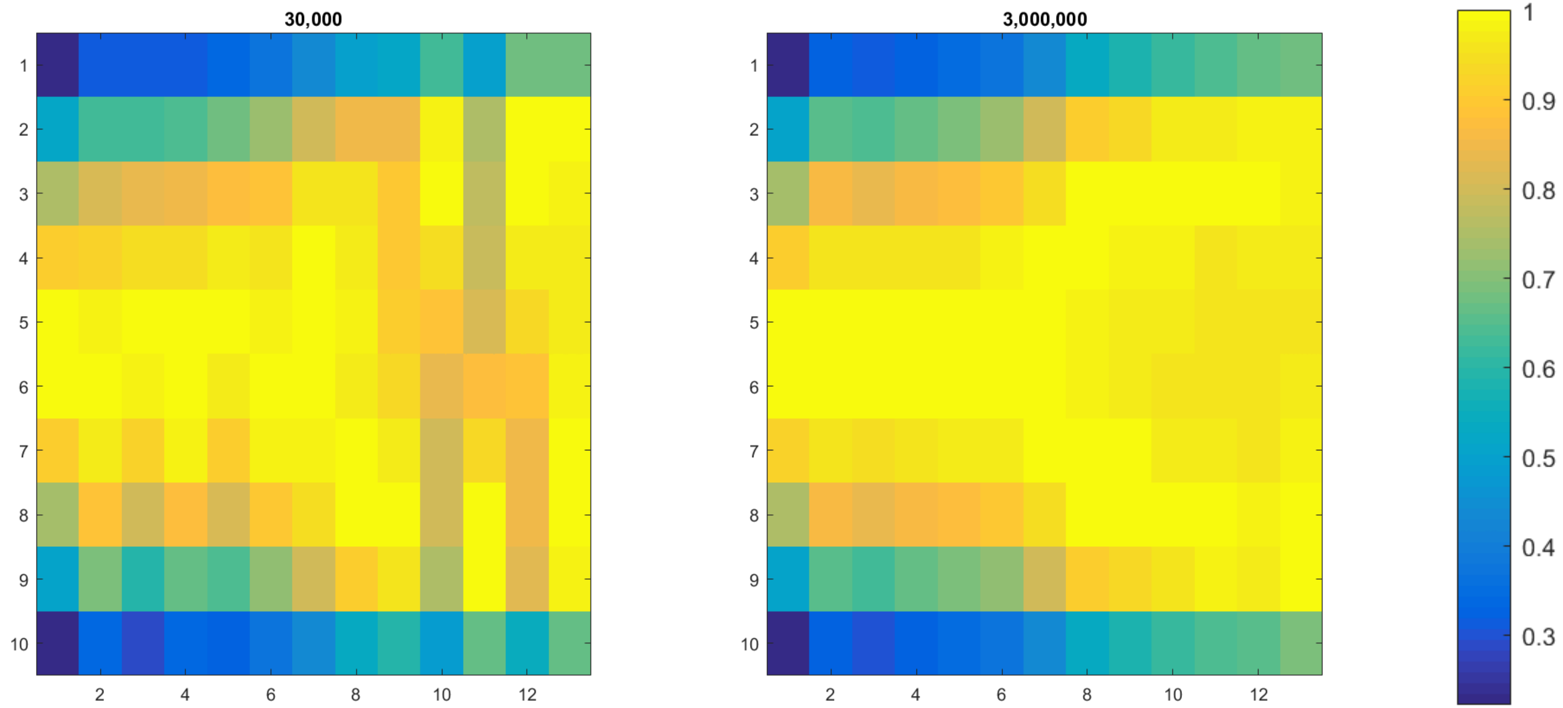
$$\epsilon = \Sigma_{i=1}^{10} \left| \frac{\phi_i}{\bar{\phi}} - \frac{1}{10} \right|$$

$$\bar{\phi} = \Sigma_{i=1}^{10} \phi_i$$



Relaxing the corrector step – CE/LI with no substeps

- Sanity check: relaxation with and without many particles per generation
- Compare 30,000/800/200 vs. 3,000,000/80/10 (accel.)



Error in the eigenvalue

❑ Choose 3 iterations, relaxation factor of 0.3 as reference: