Aalto University
School of Science
and Technology

Improved time integration methods for burnup calculations with Monte Carlo neutronics

Aarno Isotalo

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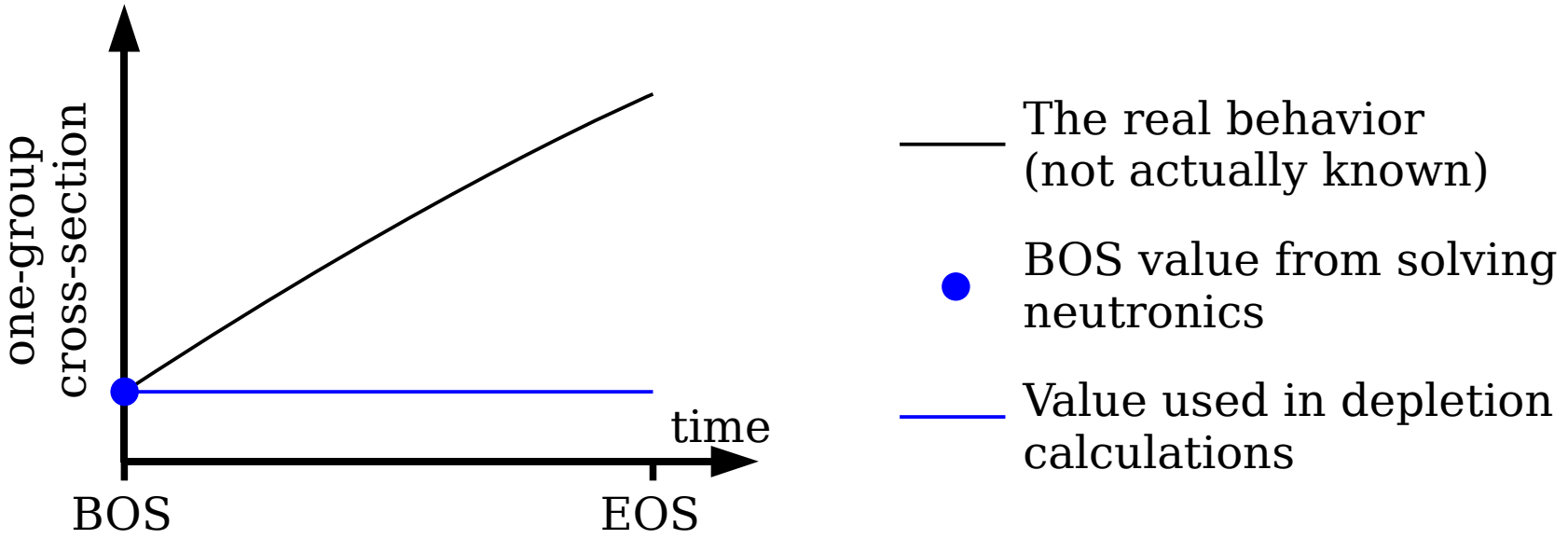
Burnup calculations

- Solving time development of reactor core parameters
  - Nuclide inventory, k_{eff}, power distribution, ...
- Two groups of methods
  - Generic ODE (Ordinary Differential Equation) solvers
  - Explicit solution of the Bateman equations with constant microscopic reaction rates for each step
    - Used especially with Monte Carlo neutronics
    - Independent neutronics and depletion solvers are combined with a wrapper algorithm
- Focus of the work: developing the wrapper algorithm
  - Largely independent of how neutronics and depletion steps are solved

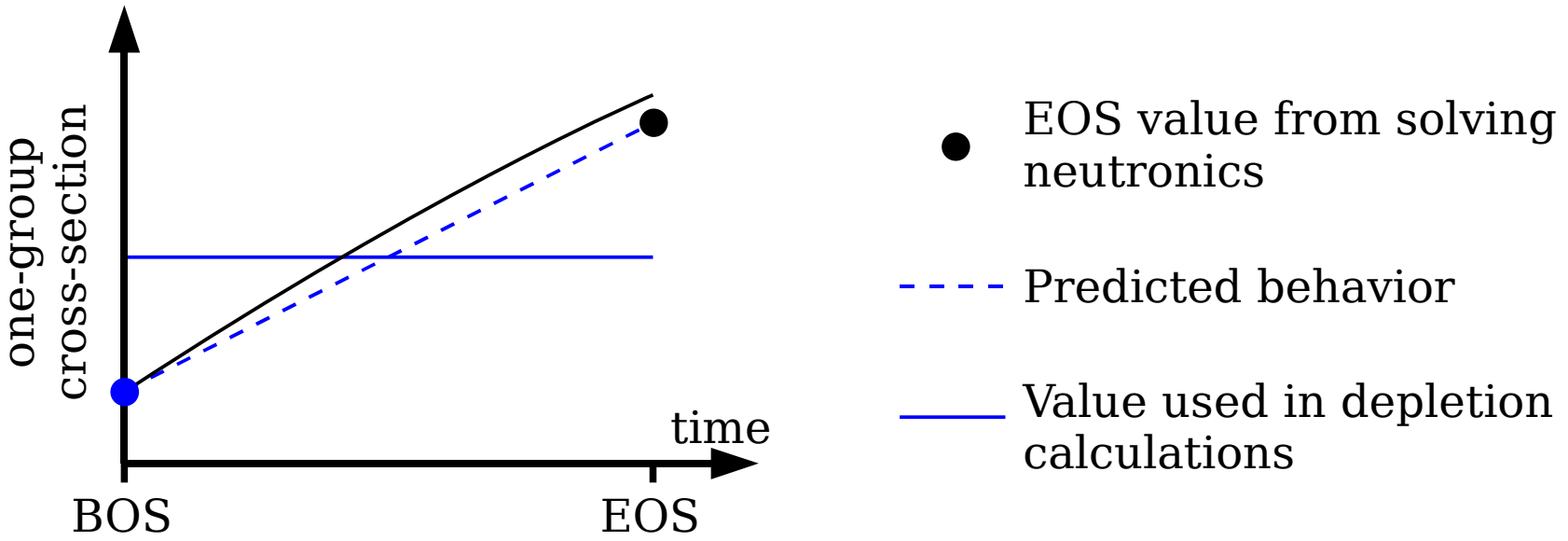
Predictor-corrector methods (1)

- Three variants, the best one (?) works as follows:
- Predictor step:
  - Solve neutronics to obtain beginning of step (BOS) reaction rates
  - Deplete with the BOS reaction rates to obtain end of step (EOS) material compositions
  - In “Euler's method” the EOS composition becomes initial composition for the next step



Predictor-corrector methods (2)

- Corrector step:
  - Solve neutronics with the predicted EOS compositions to estimate EOS cross-sections and flux
  - Redeplete using midstep/average cross-sections and flux from linear interpolation between the BOS and EOS values
  - The new EOS material compositions become the initial compositions for the next step



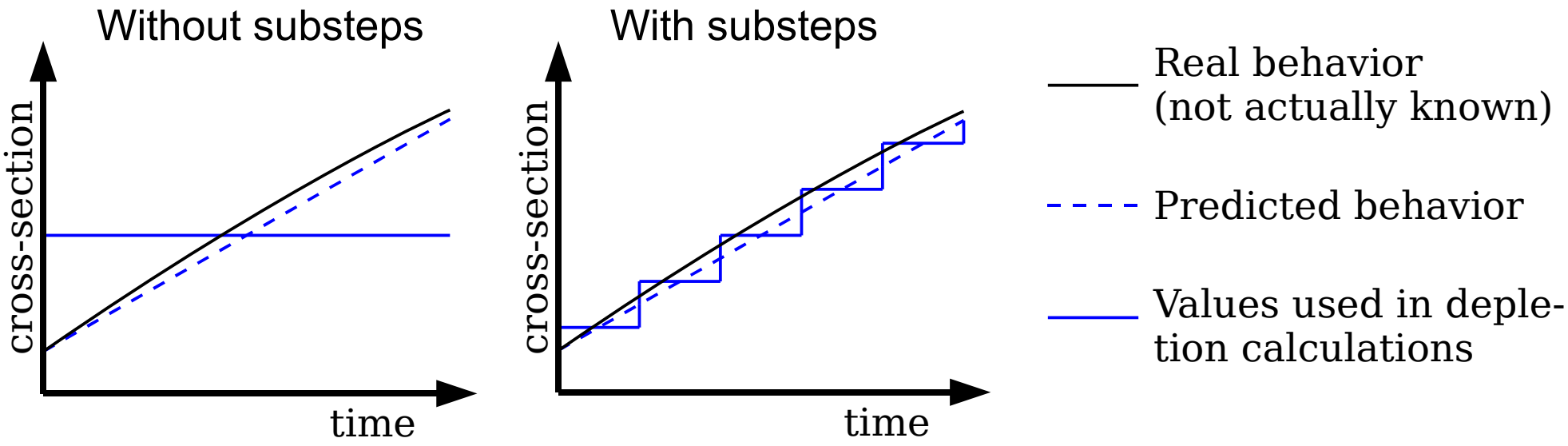
Higher order predictions

- Predictions in the traditional methods are of low order
  - Constant extrapolation on predictor
  - Linear interpolation on corrector
  - Comparable in other predictor-corrector variants
- There are no special limitations to making the predictions
- Higher order predictions using data from previous step
  - Linear extrapolation (predictor or alone)
  - Quadratic interpolation (corrector)
  - Data is recycled, no additional neutronics or depletion calculations, stepwise running time is not affected

Depletion calculations still require microscopic reaction rates to remain constant at each depletion step, but better predictions allow more representative constants to be selected.

Substeps

- Depletion steps are divided to substeps, which are solved independently
  - From constant to piecewise constant approximation
  - In this work:
    - Equal number of substeps at each step
    - Equidistant substeps
    - Average values used for each (sub)step



The tested methods

abbreviation	Predictor type	Corrector type
CE	constant	N/A
LE	linear	N/A
CE/LI	constant	linear
CE/QI	constant	quadratic
LE/LI	linear	linear
LE/QI	linear	quadratic

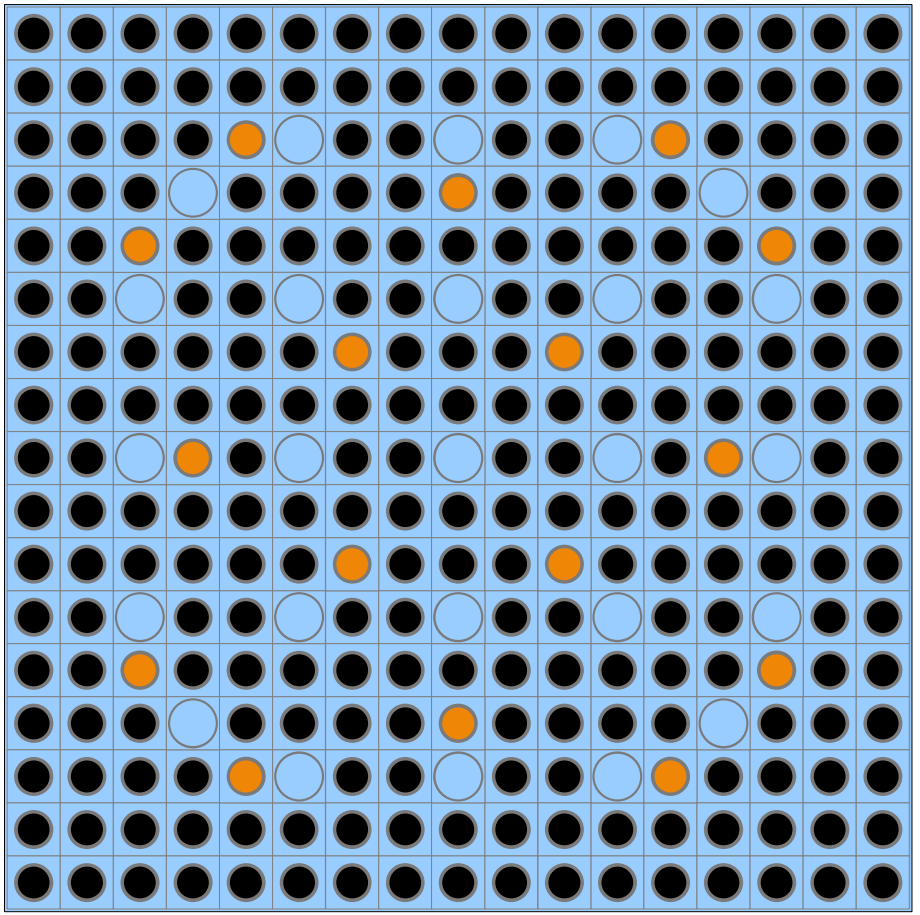
- Each can use any number of substeps (Except CE), 1 substep is equal to not using substeps at all
- CE is the old “Euler's method”
- CE/LI with 1 substep is the old predictor-corrector method

Testing

- The methods were implemented to Serpent (v. 1.1.3)
- Four test cases: 2 x assembly, 2 x pin cell
- Only the burnup algorithm differed between runs
  - Comparisons can be made as if other parts were exact
- Error from burnup algorithms controlled by step lengths
  → Reference solutions by using very short steps
- Single step methods used half as long steps as predictor-corrector methods
  - Equal running times for all methods, performance == accuracy (substeps actually cause a few % slowdown)
- Statistical variation controlled by repeating each run 5 times
  - Sample standard deviations give upper bounds for uncertainty

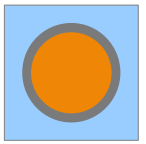
PWR assembly test case

- Westinghouse 17x17 PWR assembly
  - 16 poison rods with 3 % natural Gd

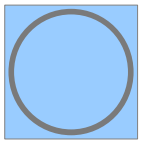


Periodic boundary conditions
Specific power: 38.6 kW/kgHM
Final burnup: 40 MWd/kgHM
Enrichment: 4.2 atom-%
Boric acid: 760 ppm

Pin cell with normal fuel rod

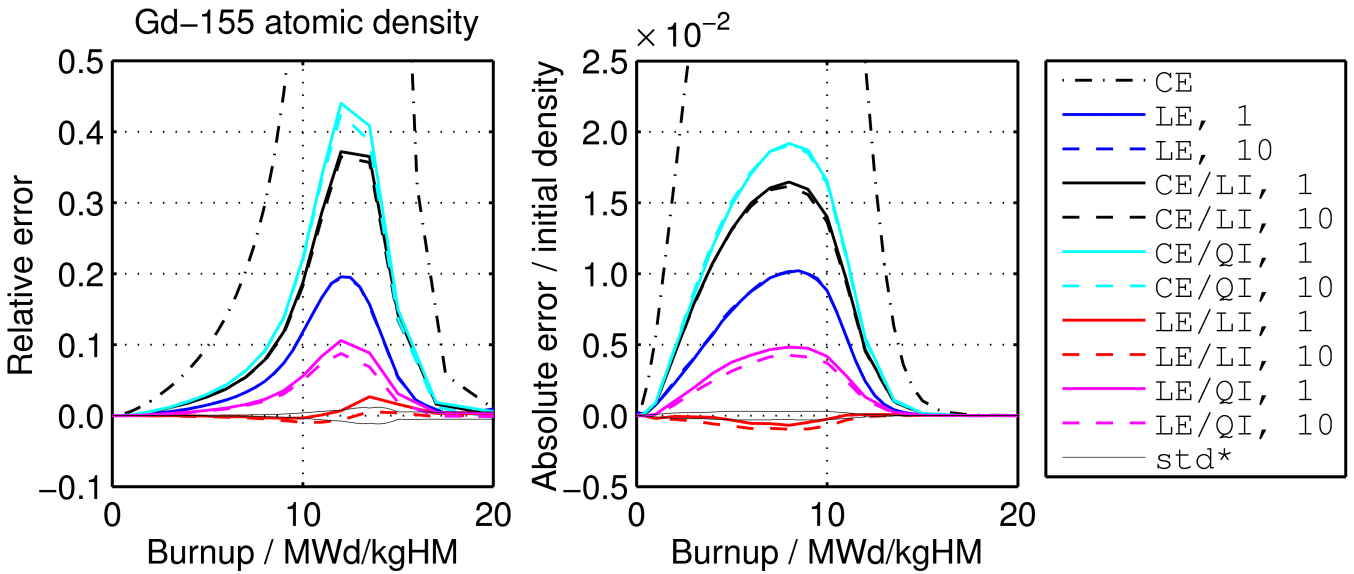


Pin cell with poisoned fuel rod



Pin cell with empty guide tube

PWR assembly results (1)

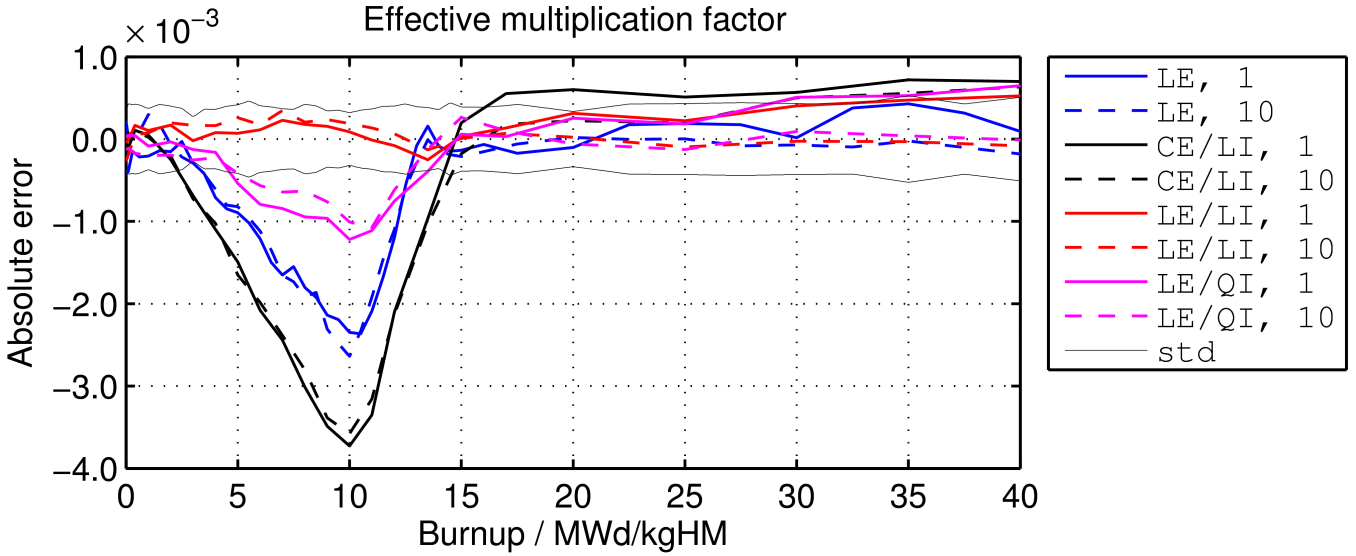


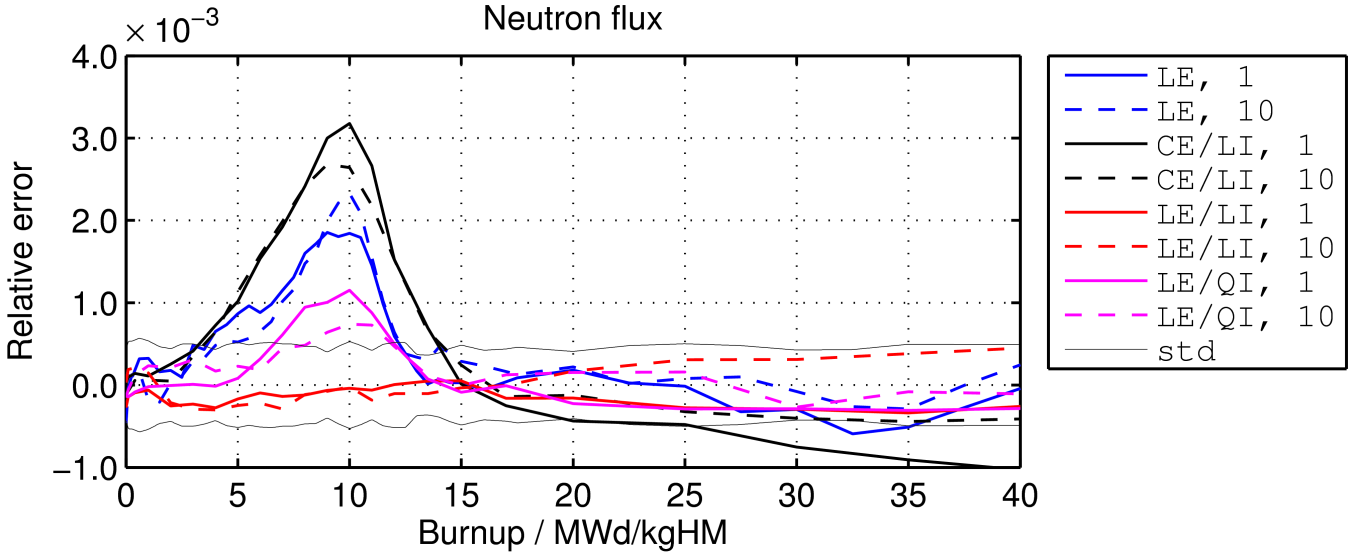
CE and LE used 43 steps
The rest used 22 steps

^{157}Gd behaves similarly, but the error peaks earlier (relative at 10 MWd/kgHM, absolute at 5 MWd/kgHM)

- CE and CE/QI were all around inferior, and have been excluded from the rest of the plots
- LE/LI relies heavily on cancellation of errors
  - Error increases with longer and shorter steps
    - Still the most accurate at all relevant step lengths

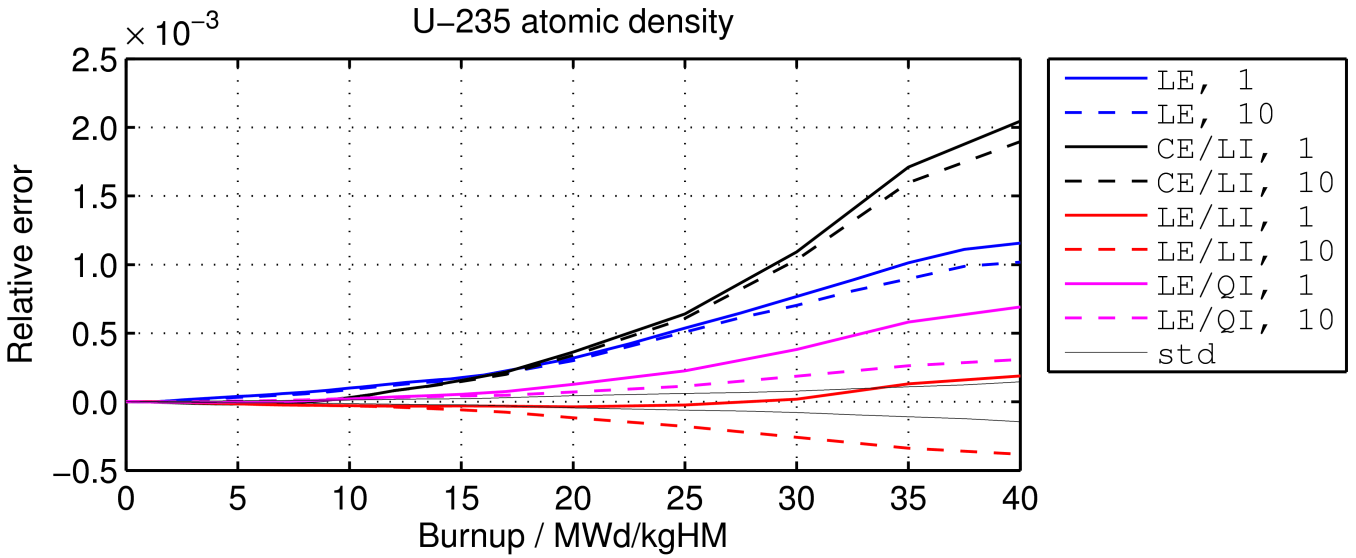
PWR assembly results (2)





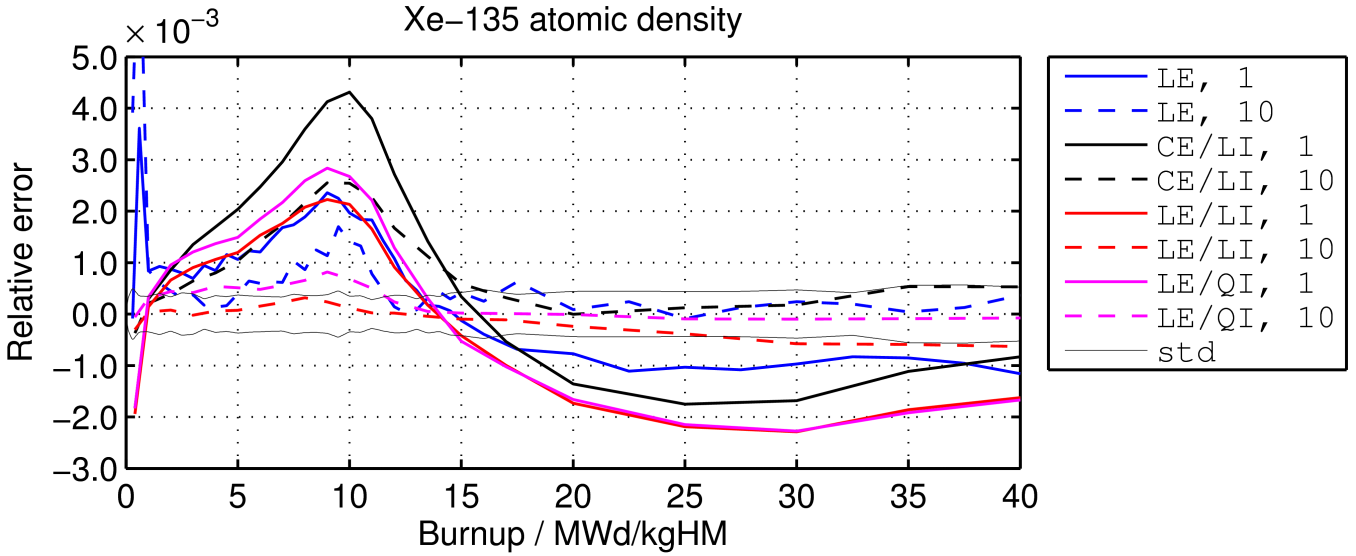
The errors in Gd are reflected by many other results

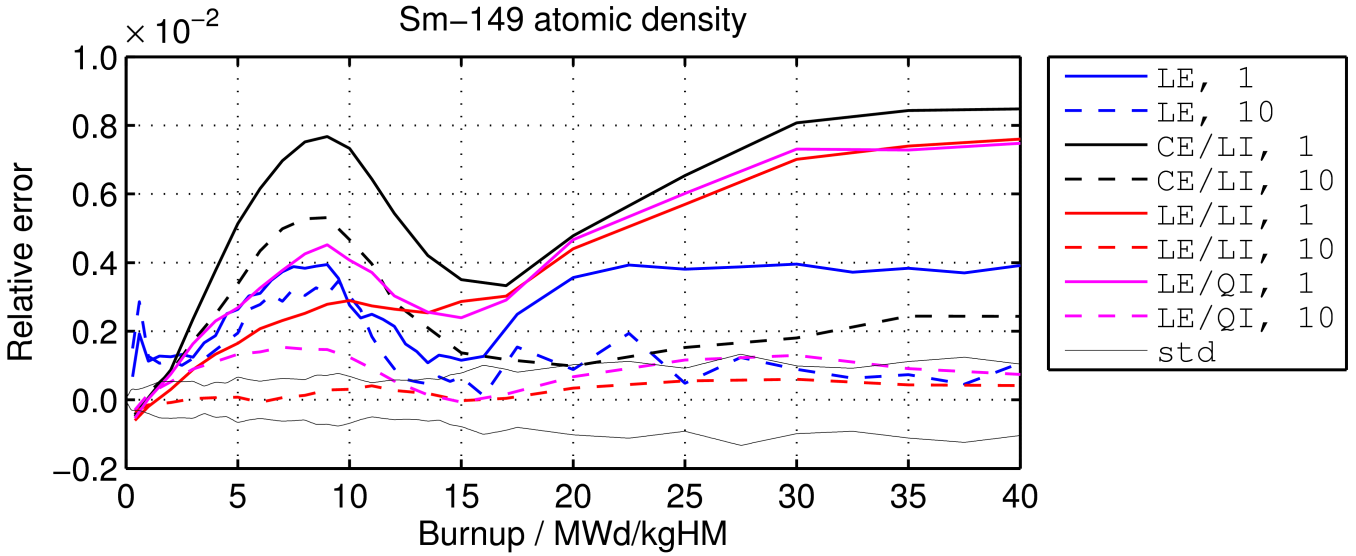
PWR assembly results (3)



- ^{235}U mostly reflects inaccuracy in the constant power normalization
  - Long-lived fission products mirror the errors in ^{235}U
- Substeps can worsen results from LE/LI
  - Reducing cancellation of errors
- The order of accuracies is similar for most other heavy metals

PWR assembly results (4)





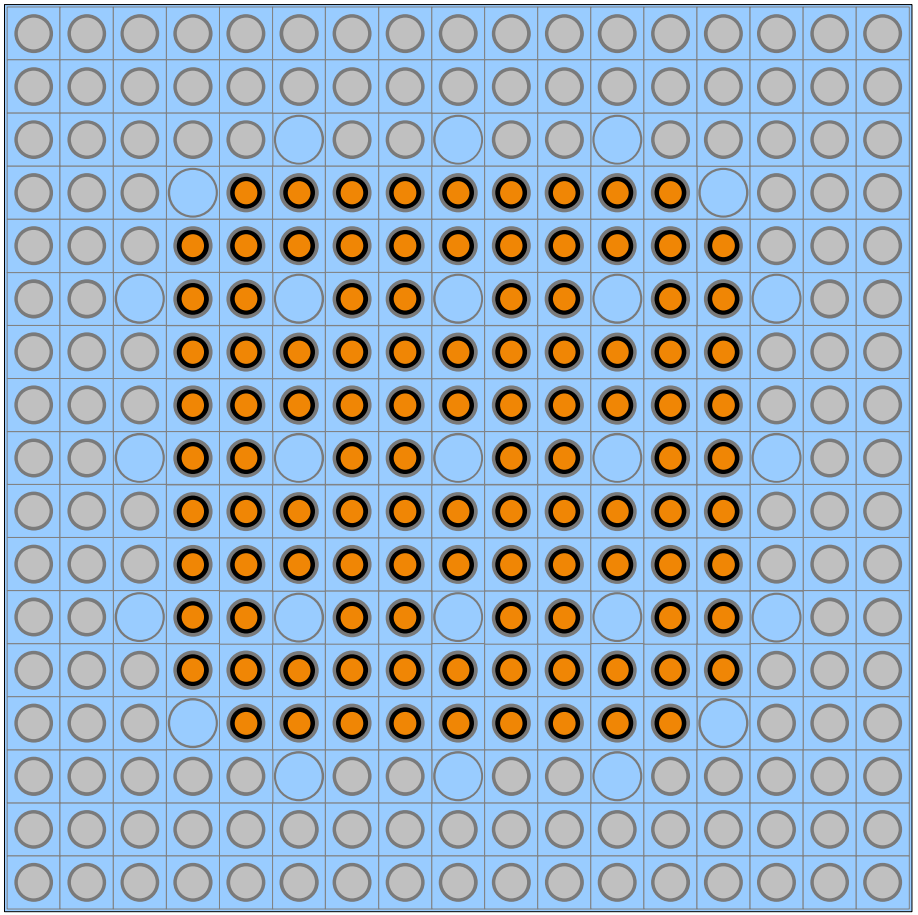
Short-lived nuclides: Error caused by EOS (secular equilibrium) concentration being calculated with average reaction rates.

Substeps shorten the discretization intervals reducing this error.

Errors in Gd concentration are also reflected by fission poisons

SBU assembly test case

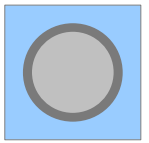
- Radkowsky thorium fuel in a seed blanket unit (SBU) configuration



Seed: 20 % enriched UO_2 surrounding
ZrO_2 plugs with 2,5 % ZrB_2

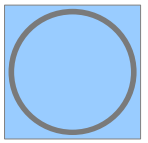
Blanket: 13 vol-% UO_2 enriched to 12.2 %
87 vol-% ThO_2

Periodic boundary conditions
Specific power: 49.07 kW/kgHM
Final burnup: 80 Mwd/kgHM
Boric acid: 760 ppm



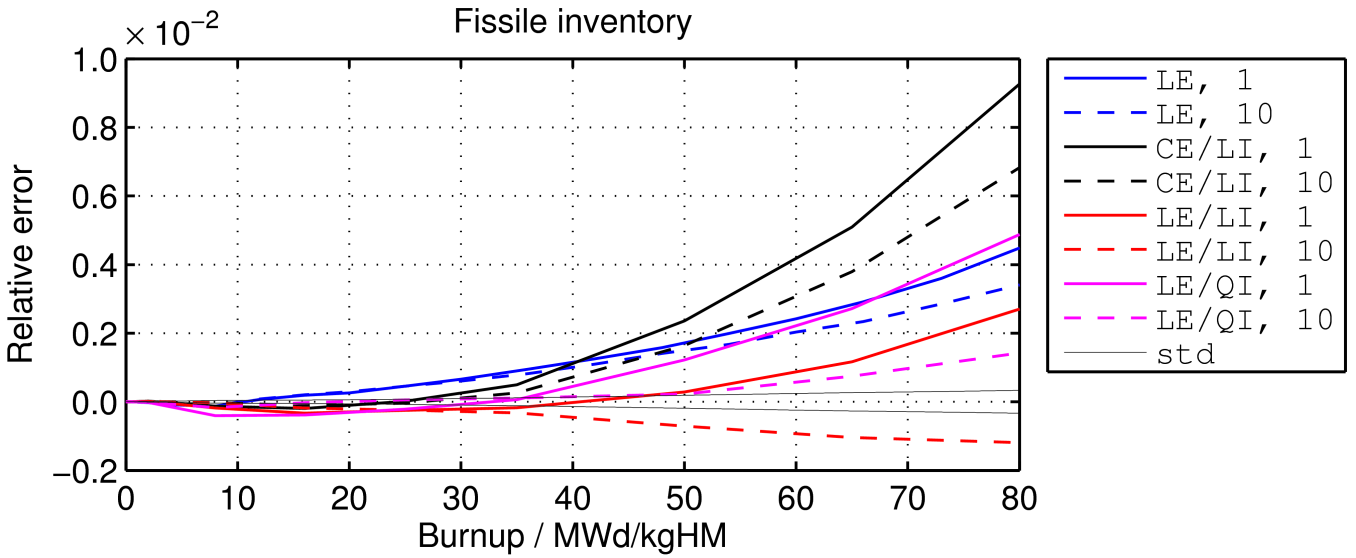
Pin cell with blanket fuel rod

Pin cell with seed fuel rod



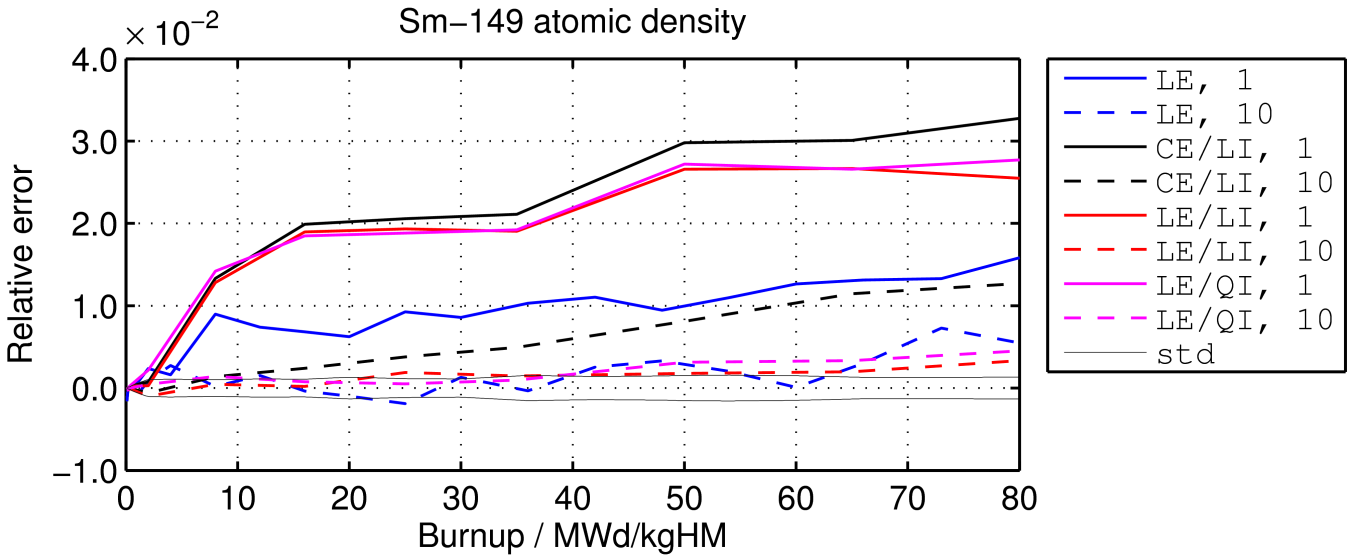
Pin cell with empty guide tube

SBU assembly results (1)



- Errors for ^{235}U, Pu and long-lived fission products behave roughly as in the PWR assembly
  - Errors in k_{eff} reflect those in the fissile inventory
- Short-lived nuclides behave as in the last half of PWR

SBU assembly results (2)



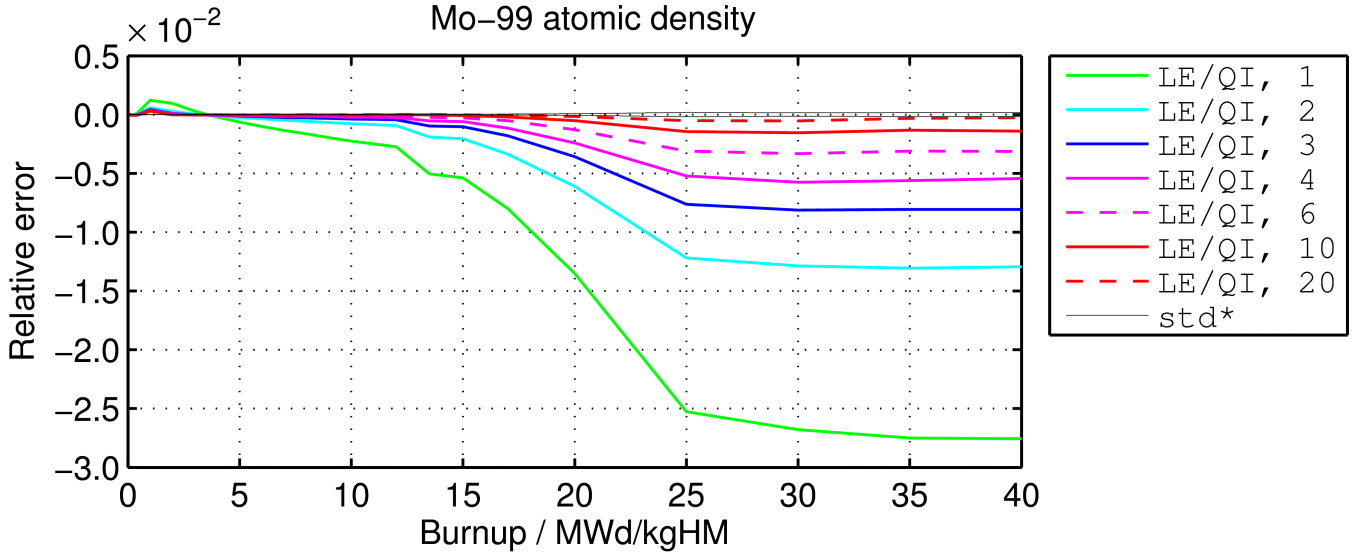
- Differences to PWR
  - Boron poison is depleted accurately by all methods even with long steps
  - The effects of predictor and corrector orders on heavy metals other than U and Pu are quite indecisive
  - Substeps have clear positive effect even on long-lived nuclides

Pin cell tests

- PWR: one normal pin cell from the PWR assembly case
  - Qualitative behavior of U, Pu, fission products roughly as above
  - Errors for non-short-lived much smaller than in the assemblies
- SFR: one core pin from Russian BN600 with MOX fuel
  - Substeps again had the same effect on short-lived nuclides
  - Errors an order of magnitude below other cases
  - No probability tables treatment in Serpent 1.1.3
- Old low orders are sufficient for such simple cases

Number of substeps

- Substeps on predictor had no noticeable effect
- Around 5 substeps on corrector are enough
  - Some short-lived fission products can benefit from more
- Substeps multiply the number of depletion calculations
  - Assembly tests 5 substeps on corrector: 4% and 2% slowdowns
  - Relative slowdown is heavily dependent on relative speeds of depletion and neutronics solutions



Conclusions

- Higher predictor order and substeps had clear positive effect
  - In the assembly test cases step lengths could be doubled
  - LE is also promising as a single step method
- Effects of quadratic interpolation on corrector were inconclusive, predominantly negative
  - Might still be preferable due to predictability
- Will be implemented to Serpent 2
- Results are not Serpent specific
  - Efficiency of substeps can vary

Thank you for your attention

Questions?