A premilinary study of the OECD/NEA 3D transport problem using the lattice code DRAGON

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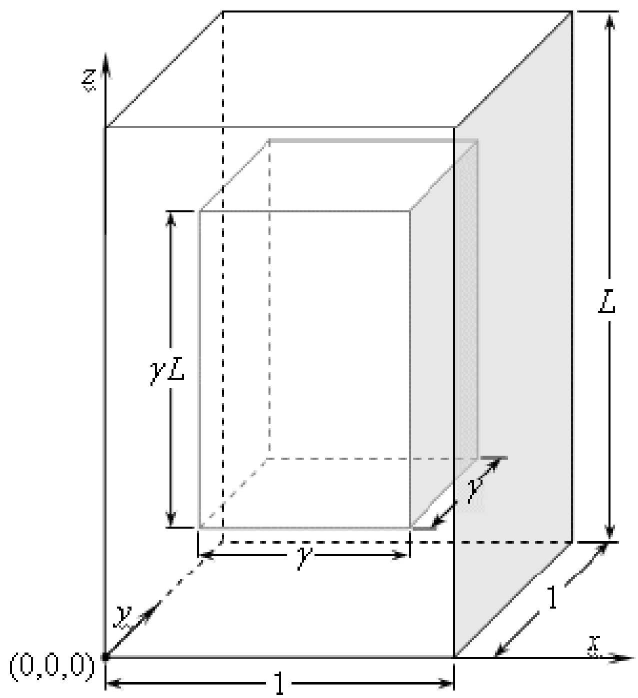
Objectives of this study

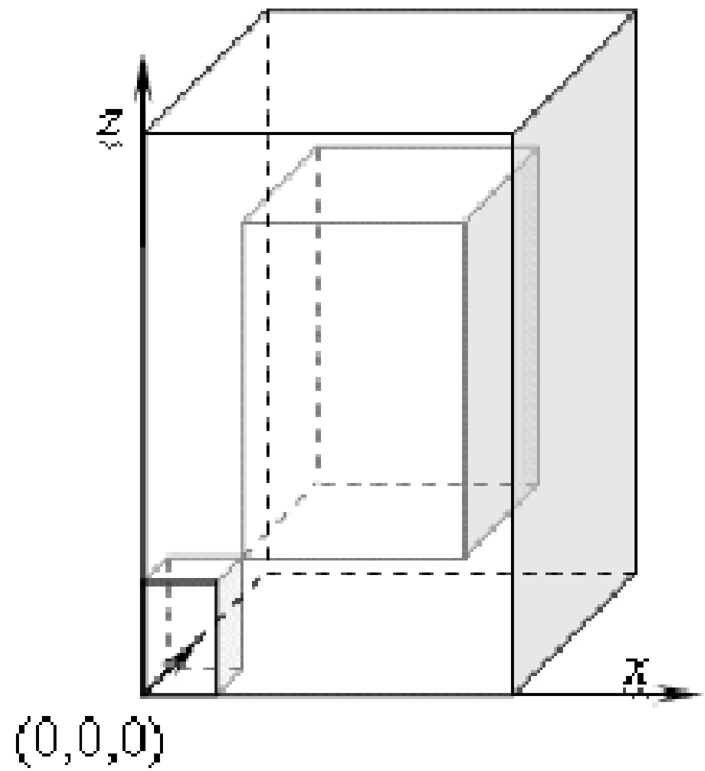
- ***To test the accuracy of 3D transport codes and methods over a range in parameter space***
  - ***Computational* benchmarks** challenge only results of 3D deterministic codes, *not* quality of the datas.
  - third's of a serie of computational benchmarks proposed by the *NEA's expert group on 3D radiative transport benchmarks*.
  - Suite of benchmarks defined by 729 configurations.
  - Observe trends towards a large variation on space parameters.
- Provide reactor physicists indications and guidelines in order to bring improvements in the numerical methods employed.

Objectives of this study

- The lattice code DRAGON can handle 3D neutron transport problems using the :
  - Collision probabilities (CP) method.
  - Caracteristics method (CM).
  - Discrete ordinates (S_N) method.
- S_N and MOC solutions have been produced (no CP solutions).
- *Verification* of the code vs. MCNP reference solutions.
  - Especially, verification of the recent extention of the **SNT:** module to 3D Cartesian geometries.
- Comparison with other deterministic codes.
- If possible, determine shortcomings of DRAGON's implementation of these numerical methods.

Presentation the benchmark





- Source dimension of $(1-\gamma/2)\times(1-\gamma/2)\times L(1-\gamma/2)$
- $6\times 6\times 6$ regions, x-y co-ordinates: $\left\{0, \frac{1-\gamma}{4}, \frac{1-\gamma}{2}, \frac{1}{2}, \frac{1+\gamma}{2}, \frac{3+\gamma}{4}, 1\right\}$ and z=$L\times\{x$ or $y\}$

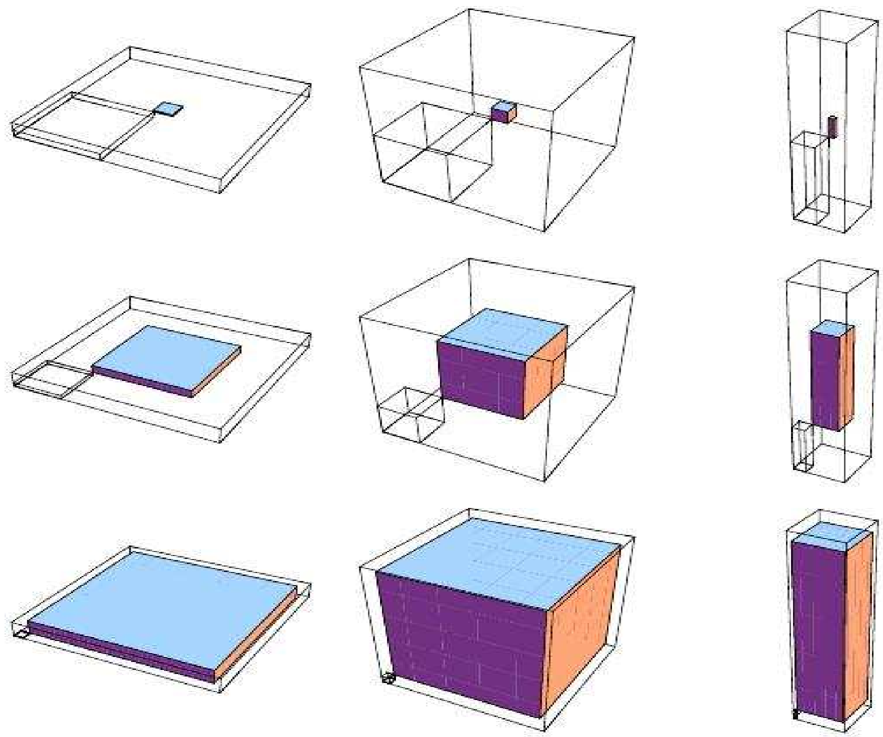
Parameters:

- Variation of
  - L, length of the outer parallelepiped (1)
  - γ, scaling factor between parallelepiped (2) and (1)
  - Σ_1, total cross-section of (1)
  - c_1, scattering ratio ($\frac{\Sigma_s}{\Sigma_t}$) of (1)
  - Σ_2, total cross-section of (1)
  - c_2, scattering ratio ($\frac{\Sigma_s}{\Sigma_t}$) of (2)

Parameters	Values		
L	0.1	1.0	5.0
γ	0.1	0.5	0.9
Σ_1	0.1	1.0	5.0
c_1	0.5	0.8	1.0
Σ_2	0.1	1.0	5.0
c_2	0.5	0.8	1.0

- **3 possible values for each quantity** $\Rightarrow 3^6 = \mathbf{729}$ **configurations.**
- **mean free path vary to** $0.1 \times 0.1 \times 0.01$ **to** $5 \times 5 \times 25$ **mfp.**
- **Required values:**
  - **scalar fluxes computed over 15 subvolumes.**
  - **Net leakage out over 8 sufaces.**
- Configurations identified as “abcdef”,*i.e.*, 111111 and 333333 resp. first and third column.

Resulting geometries: 1



- L vary by column: $L = [0.1; 1.0; 5.0]$.
- γ by row: $\gamma = [0.1; 0.5; 0.9]$

Computational strategy in DRAGON 1

- Two complete solutions proposed, using 2 different methods:
  - Discrete ordinates (S_N) method.
  - Method of characteristics (MOC).
- premilinary parametric study done for both methods:
  - 3 sets of spatial and angular discretizations per solution
  - Error should theorically decrease by refining the computational model (*asymptotic regime*)
  - But in some cases, strong coupling between space and angular variables raise limitations of the discretization approach (ray effect, numerical diffusion, negative fluxes...).

S_N computational strategy

- First study:
  - Parabolic Diamond-Differencing scheme.
  - Uniform spatial discretization of the regular geometry by $subm$.
  - S_n Level-symmetric quadrature (LQ_n), $n \leq 20$.
  - DSA-preconditionning and $GMRES(10)$ acceleration of the inner iterations.
  - $$[subm; S_n] = \{[2, S_{16}]; [3, S_{18}]; [4, S_{20}]\}$$
- Recent developments in DRAGON allow us to use (both for **SNT:** or **NXT:** tracking operators):
  - Legendre-Chebyshev quadrature (P_n-T_n), $n \leq 44$.
  - Quadruple-Range quadrature (QR_n), $n \leq 74$.

MOC computational strategy 1

- Diamond Differencing scheme along the tracking lines.
- Self-collision rebalancing (SCR) acceleration of inner iterations.
- $GMRES(10)$ Krylov Subspace method for accelerating SCR preconditionned inner iteration.

Tracking options:

- Uniform discretization of the geometry by a factor of $subm$.
- Track density ρ (density of integration lines in cm^{-2}).
- Angular quadrature of type P_n-T_n with $nangl$.

$$[subm; \rho, nangl] = \{[2, 5 \times 10^2, 16]; [3, 5 \times 10^2, 24]; [4, 1 \times 10^3, 32]\}$$

Display of the results

- Mean relative error by case:

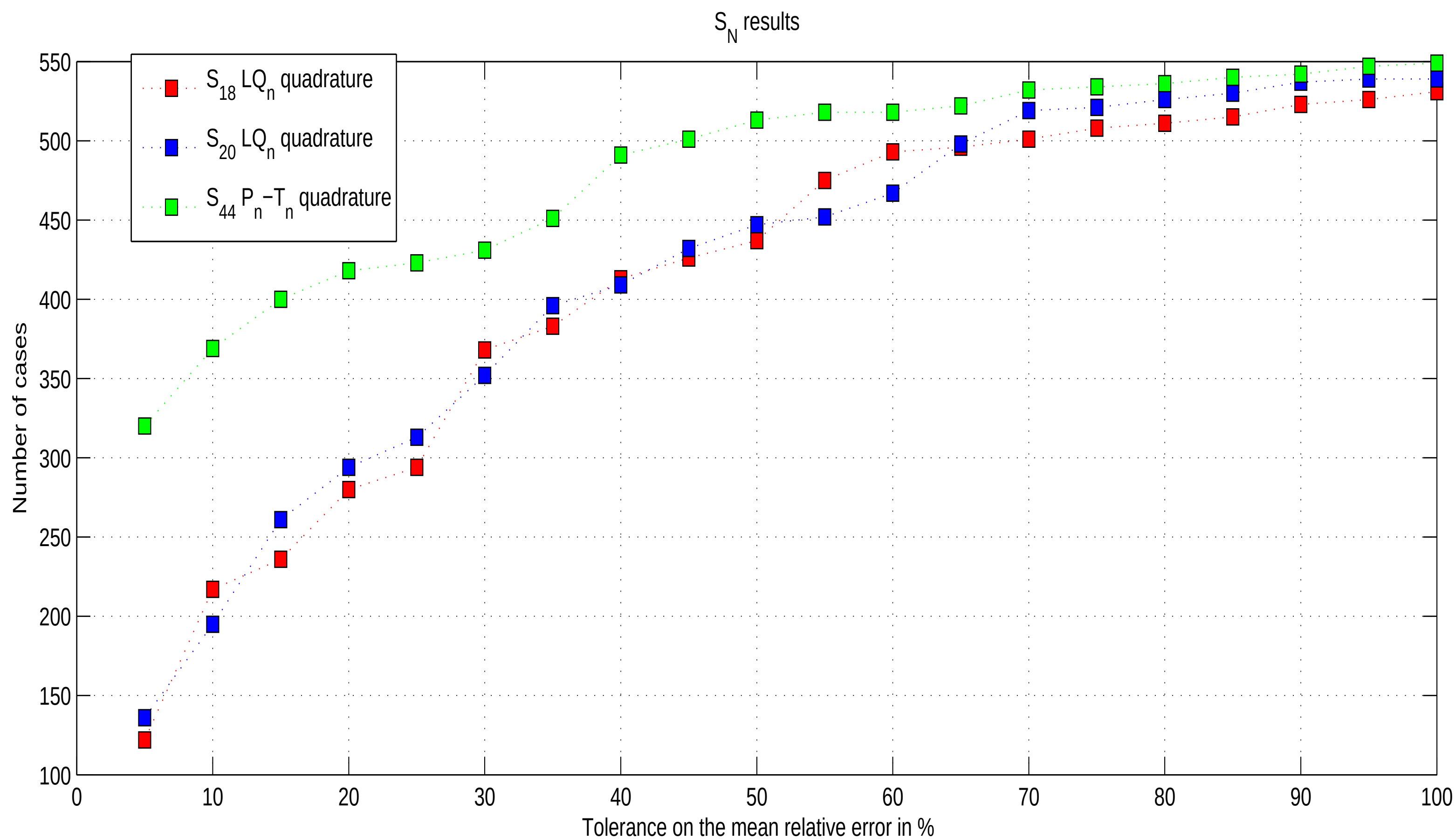
$$\delta_n(\%) = \frac{1}{N_r}\sum_{i=1}^{N_r}\frac{\Phi^i_{\text{DRAGON}} - \Phi^i_{\text{MCNP}}}{\Phi^i_{\text{MCNP}}}$$

- Total number of cases n that satisfy a criterion on the mean relative error:

$$\delta_n \leq \epsilon$$

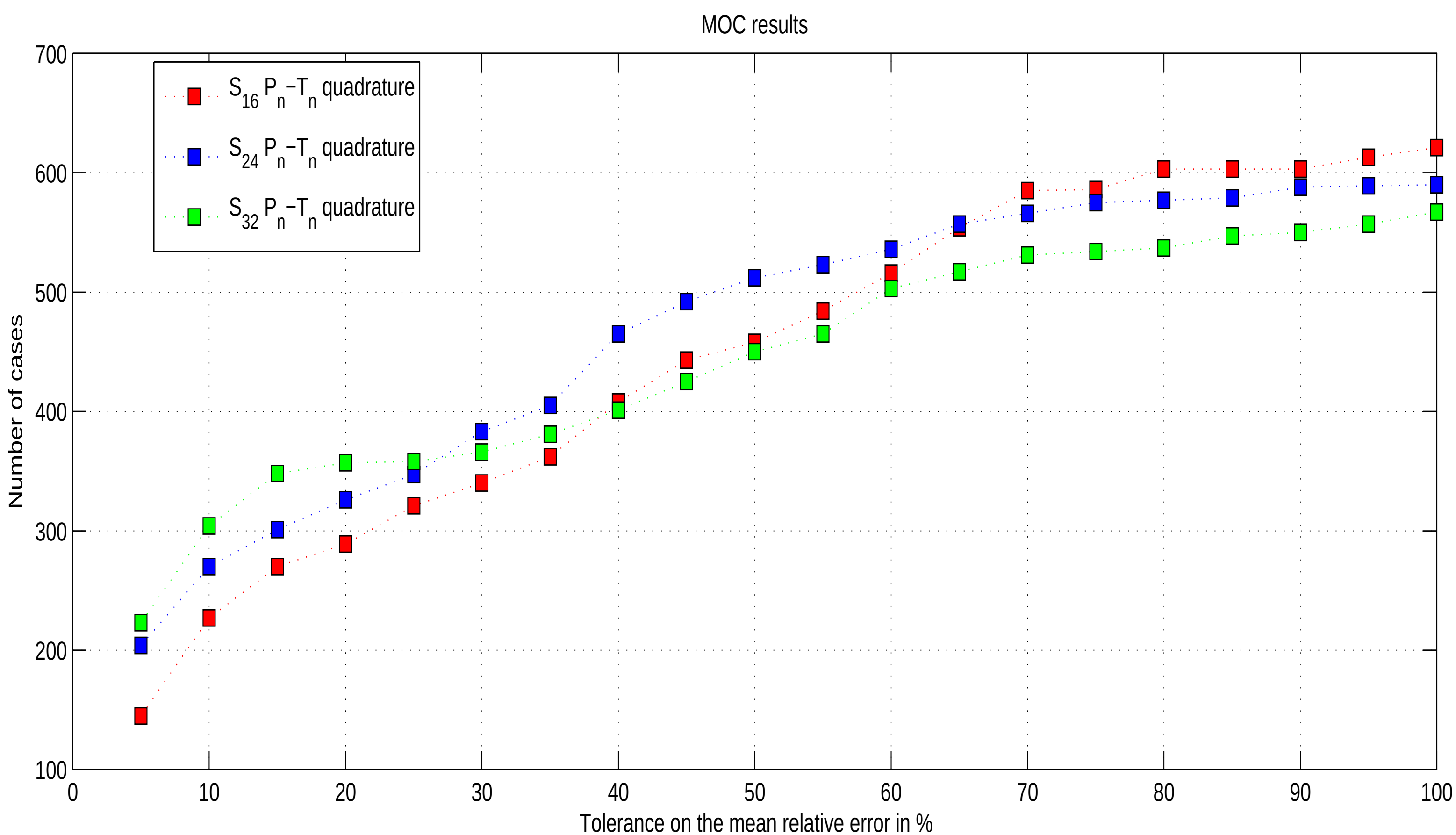
with ϵ a tolerance on the mean relative error in %.

Cumulative distribution of S_N results



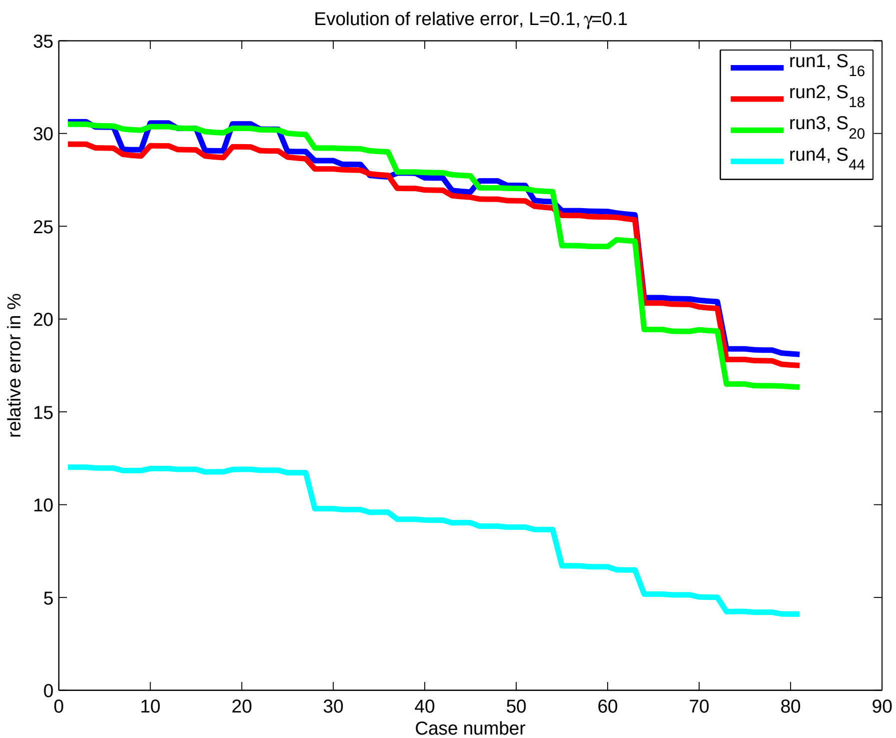
- Show the impact of the quadrature order (LQ_n quadratures are clearly inadequate).

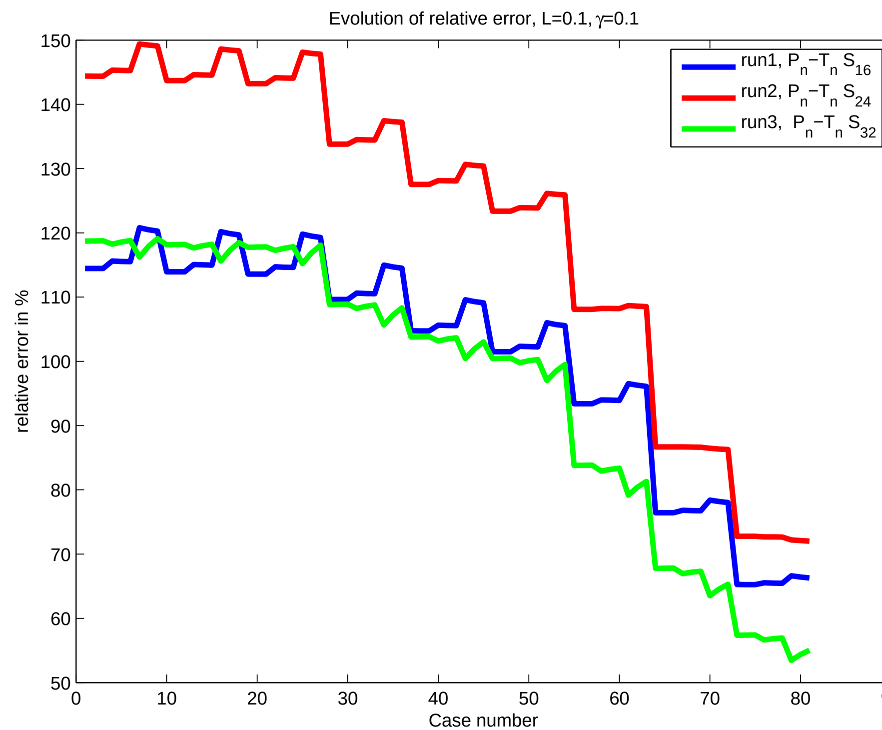
Cumulative distribution of MOC results 1

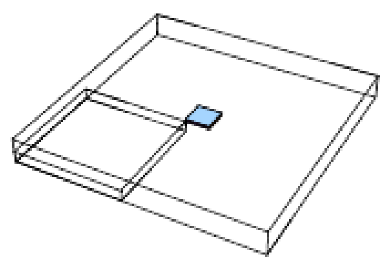


- Less impact of the angular order, but difficulty to reach mean relative error lower than 5 %.

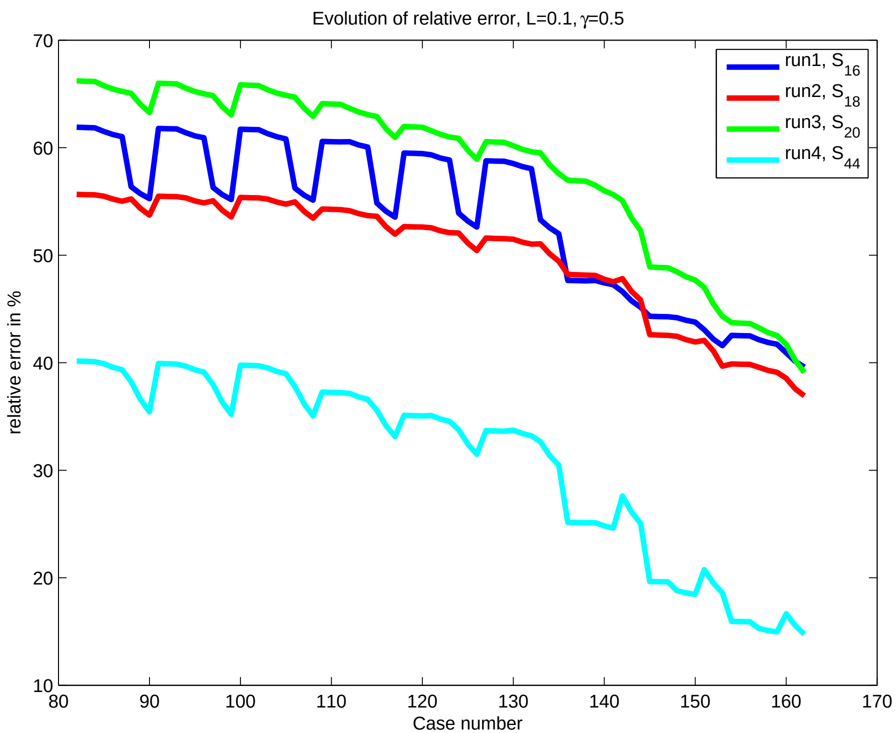
Results for $L = 0.1 \& \gamma = 0.1$

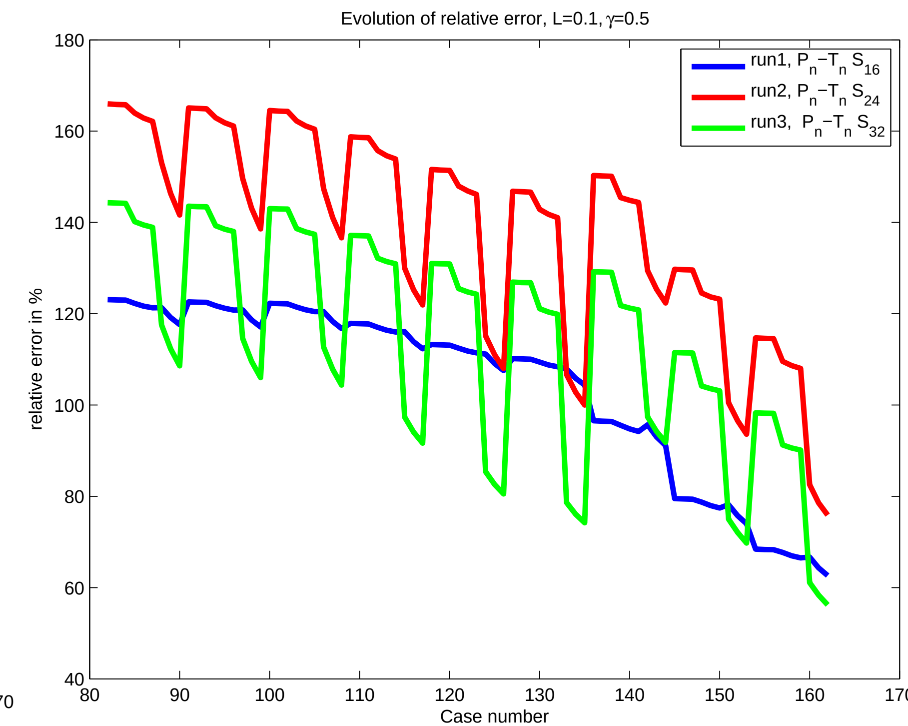


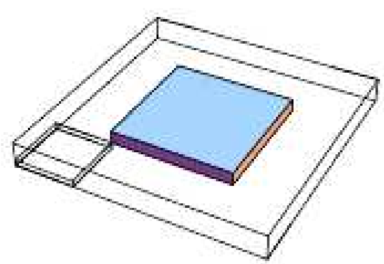




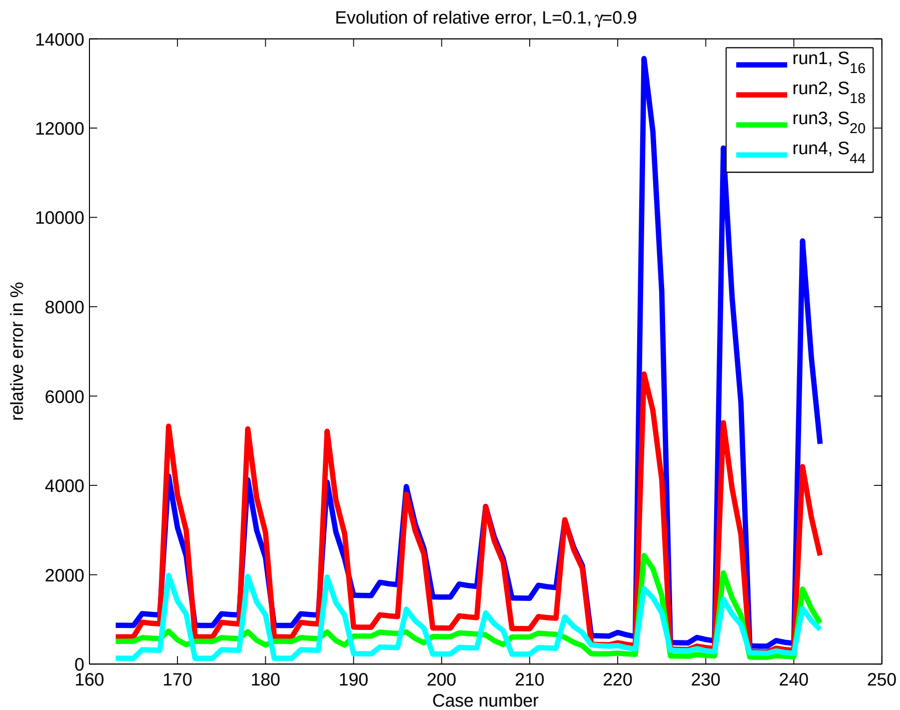
Results for $L = 0.1 \& \gamma = 0.5$

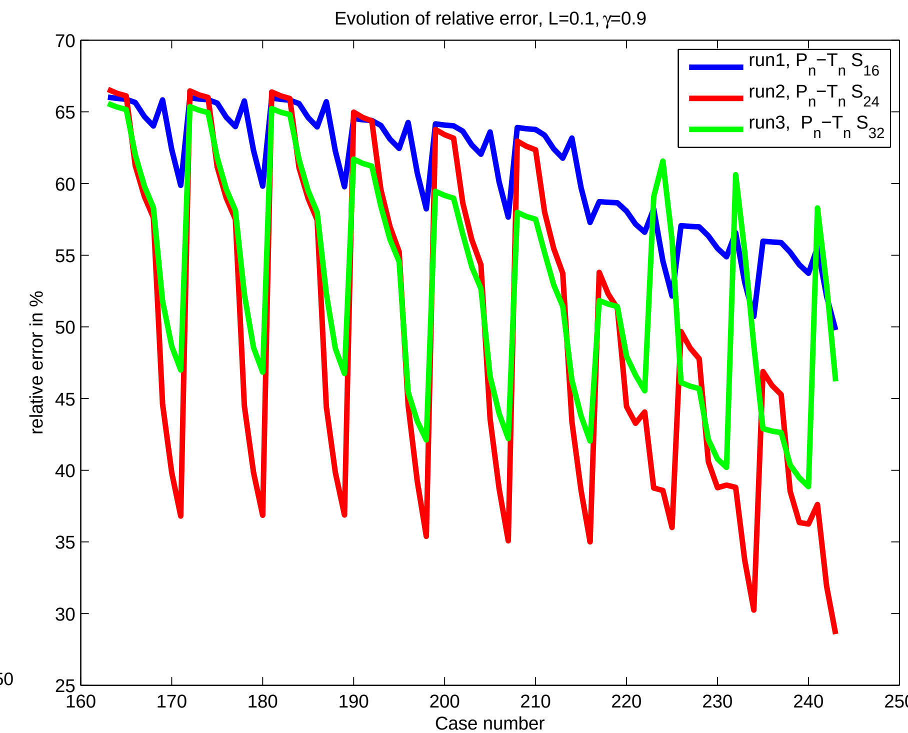


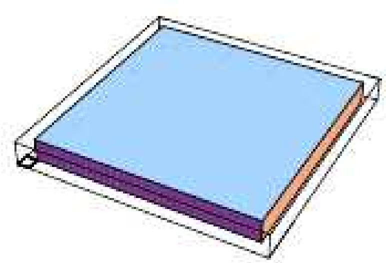




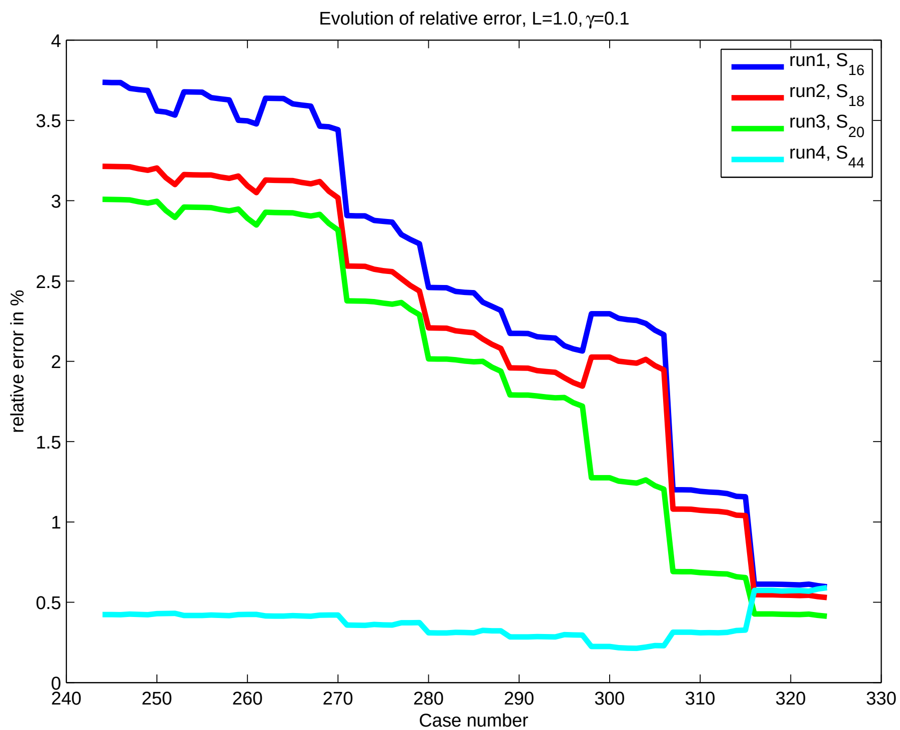
Results for $L = 0.1$ & $\gamma = 0.9$

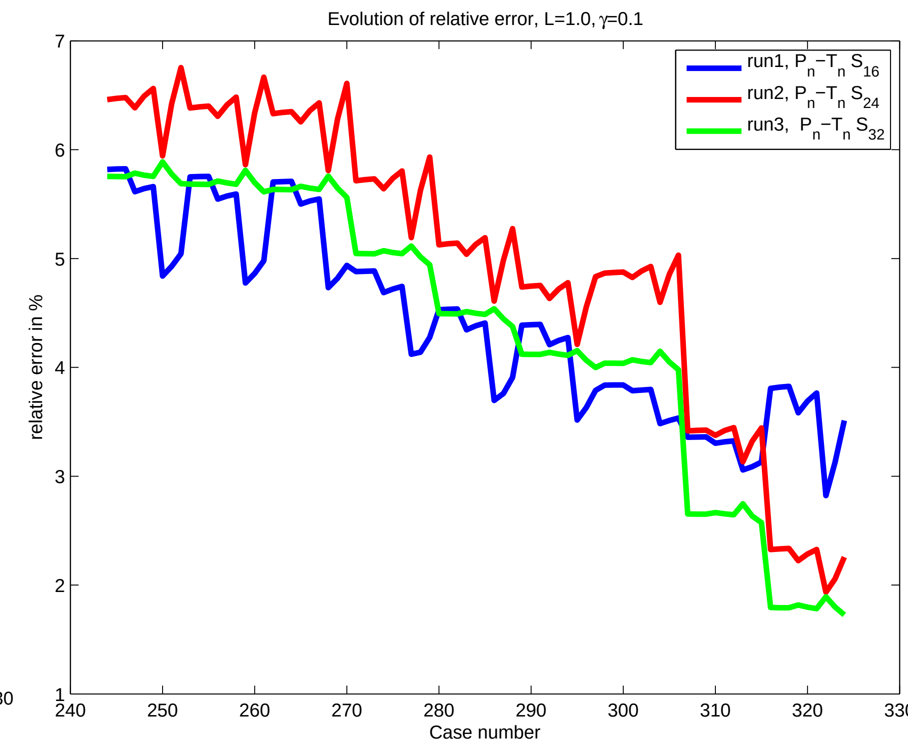


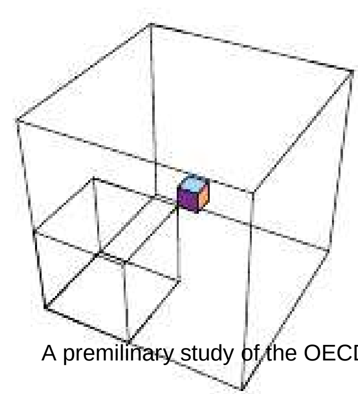




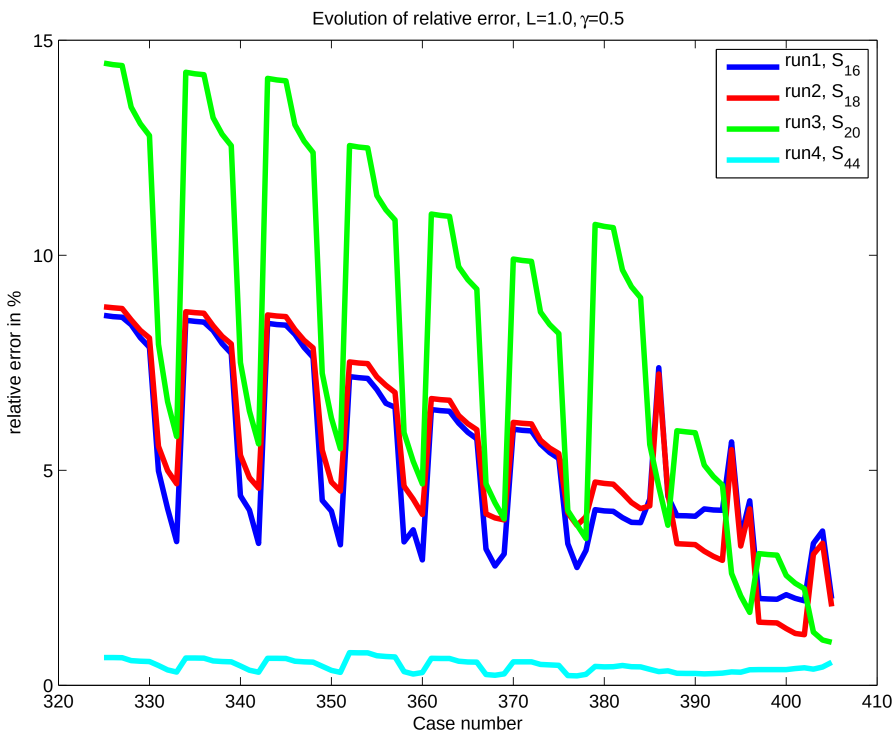
Results for $L = 1.0 \& \gamma = 0.1$ 1

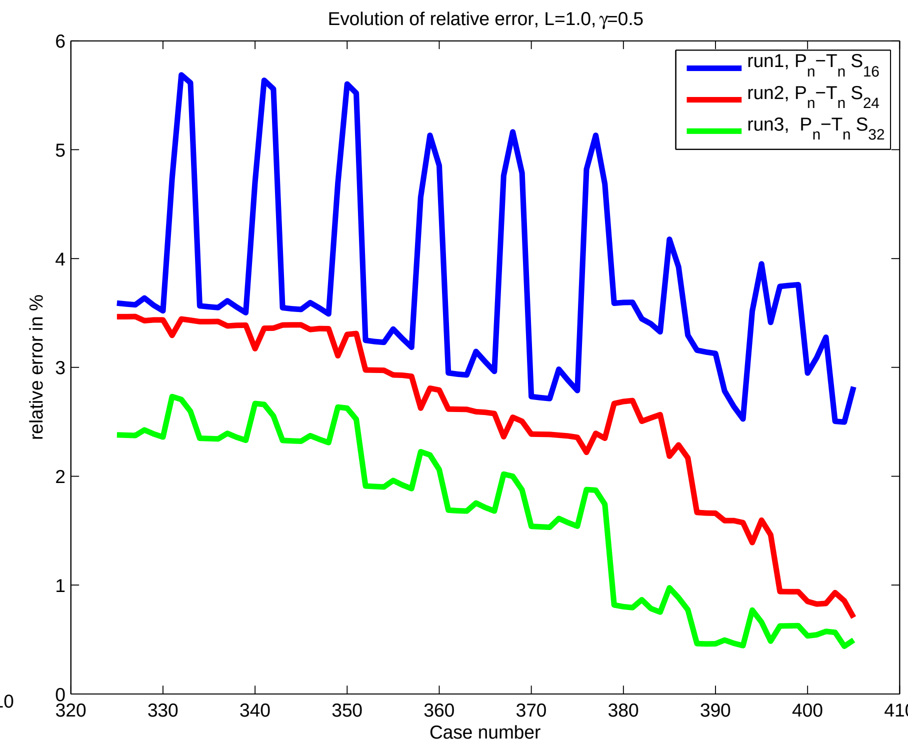


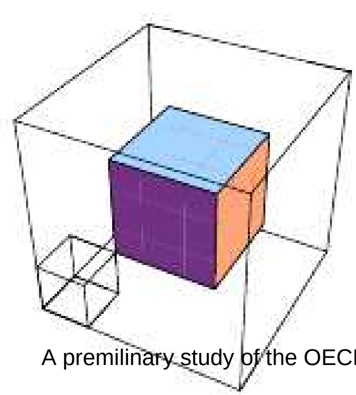




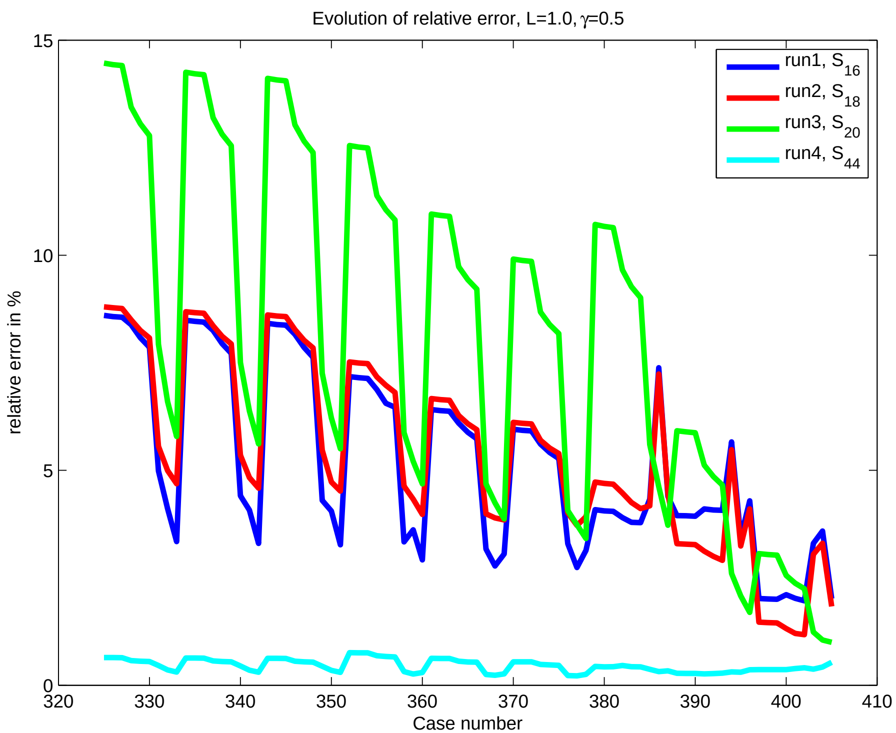
Results for $\mathbf{L = 1.0 \& \gamma = 0.5}$ 1

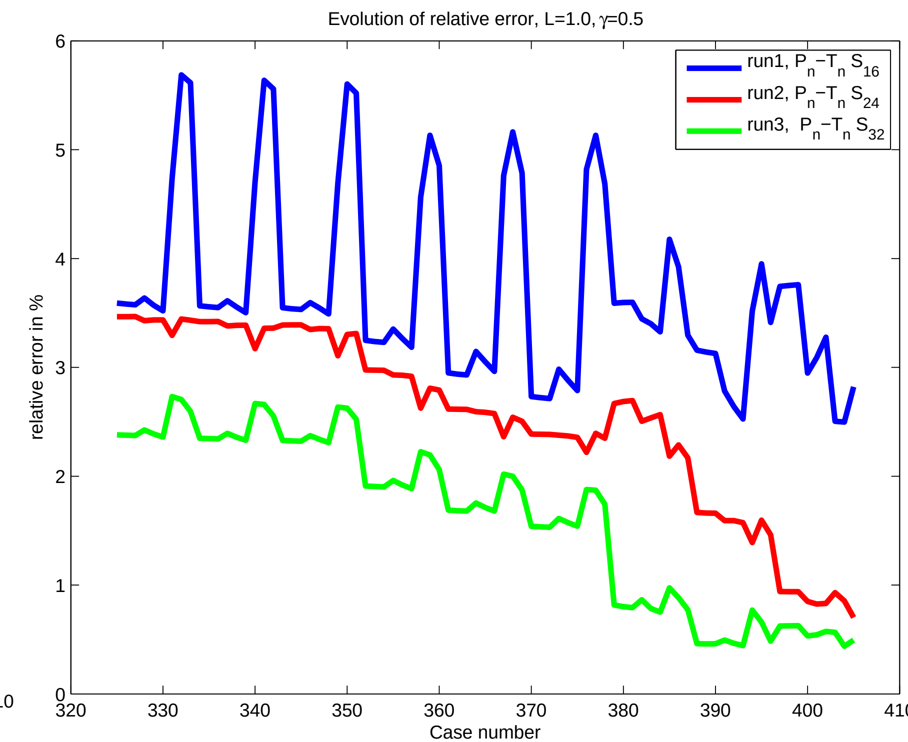


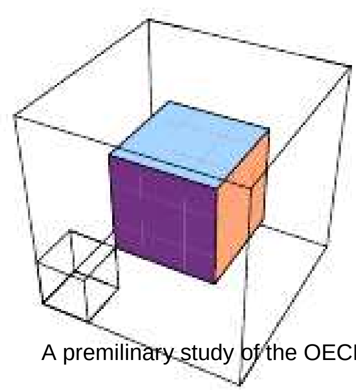




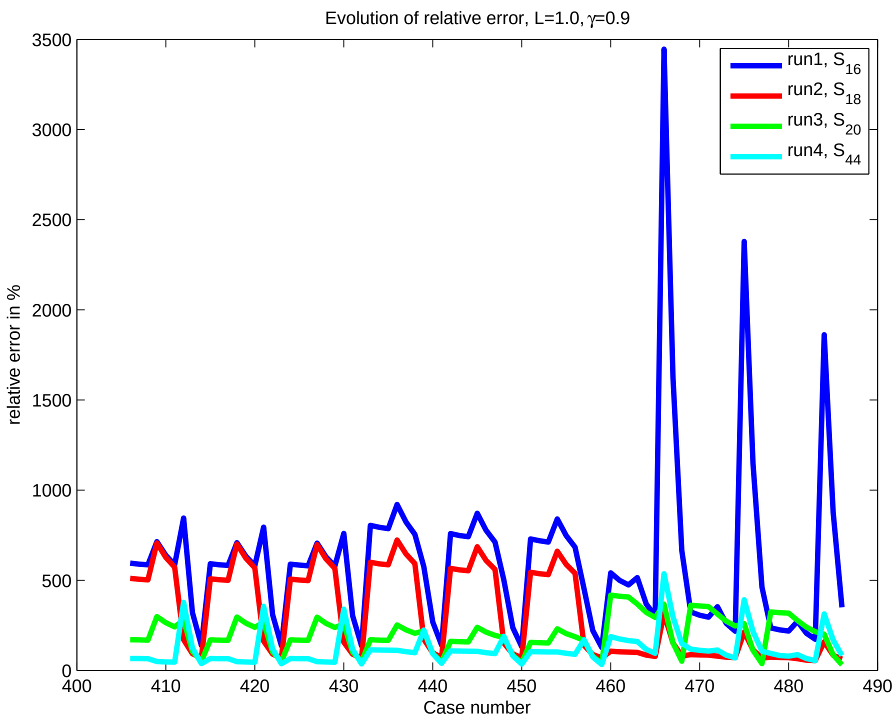
Results for $\mathbf{L = 1.0 \& \gamma = 0.9}$

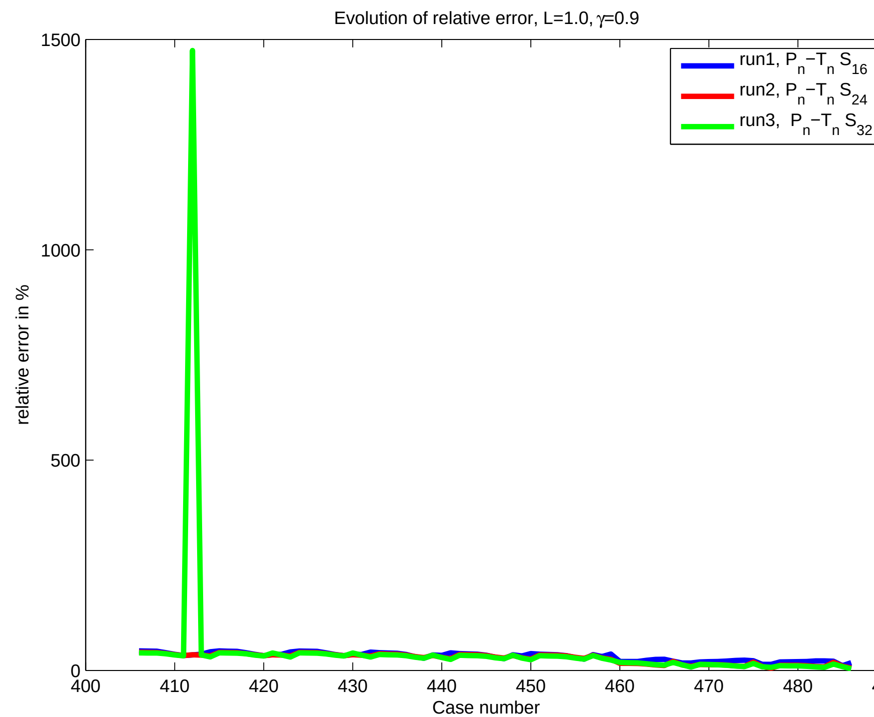


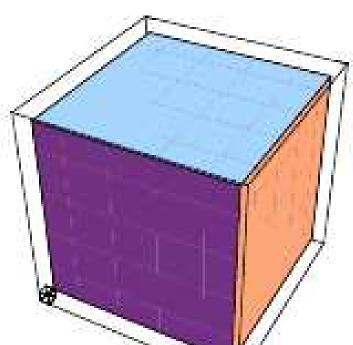




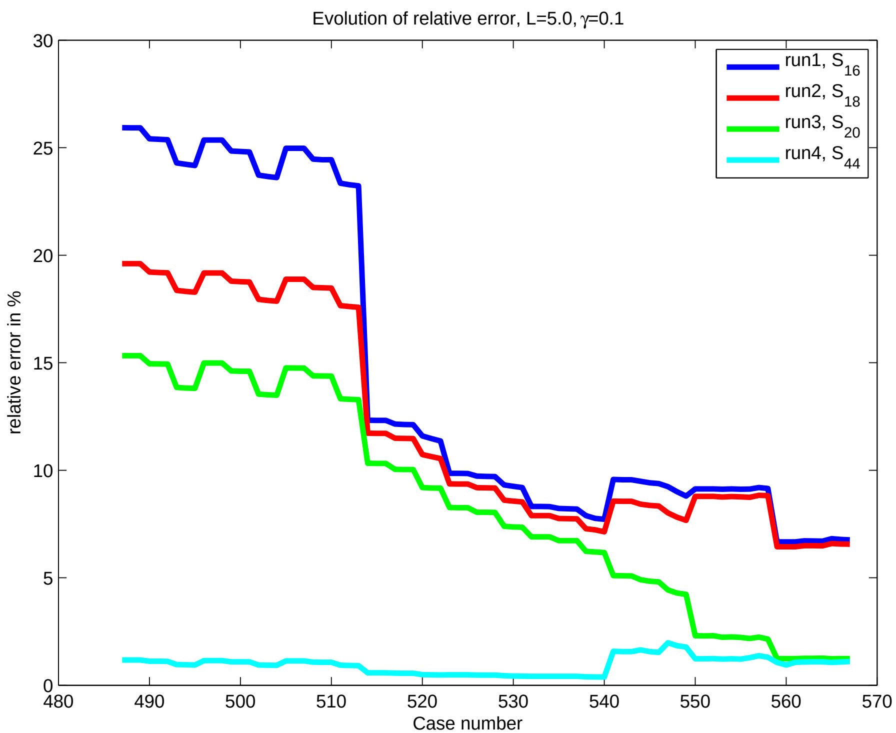
Results for L $= 1.0 \& \gamma = 0.9$

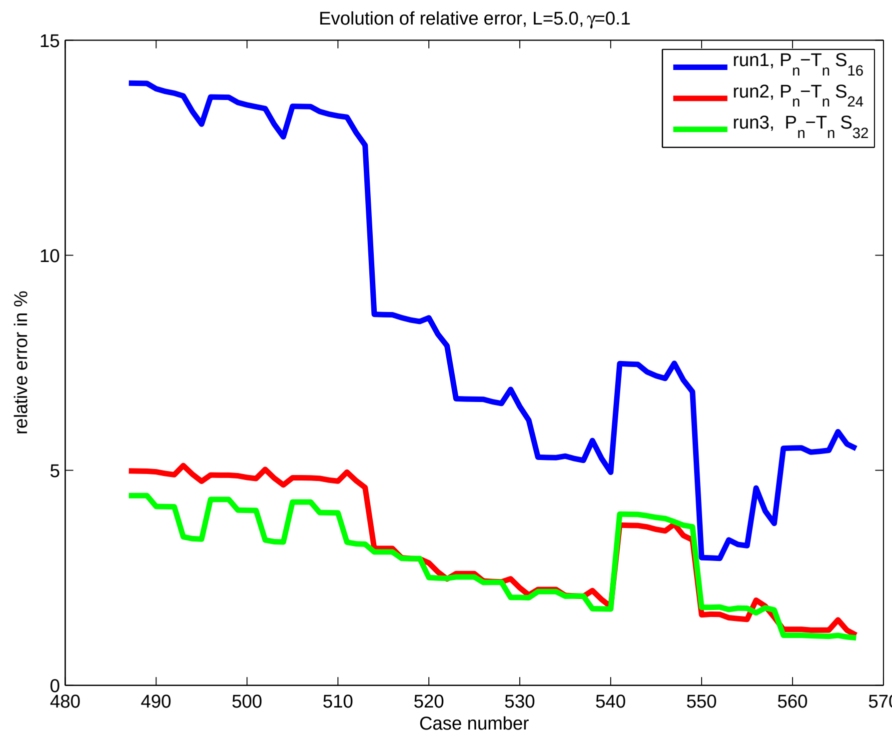


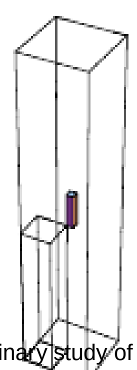




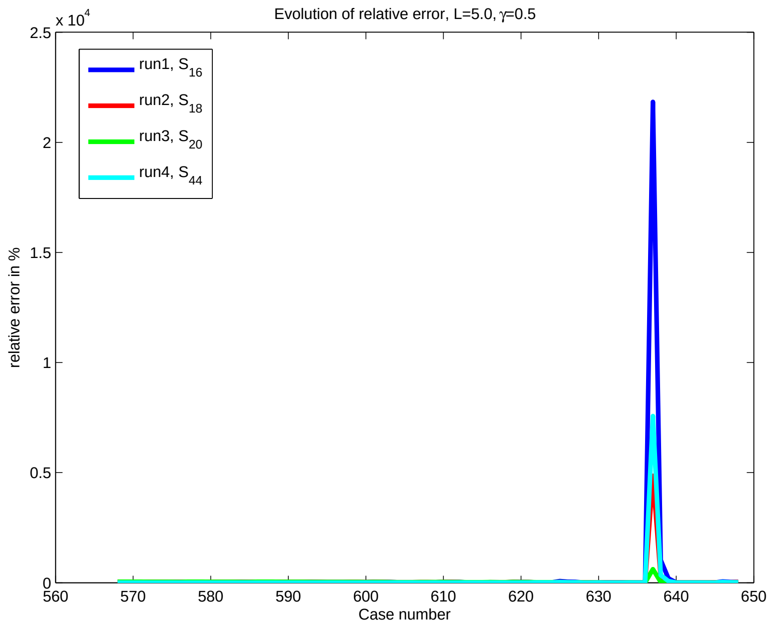
Results for $\mathrm{L} = 5.0 \& \gamma = 0.1$ 1

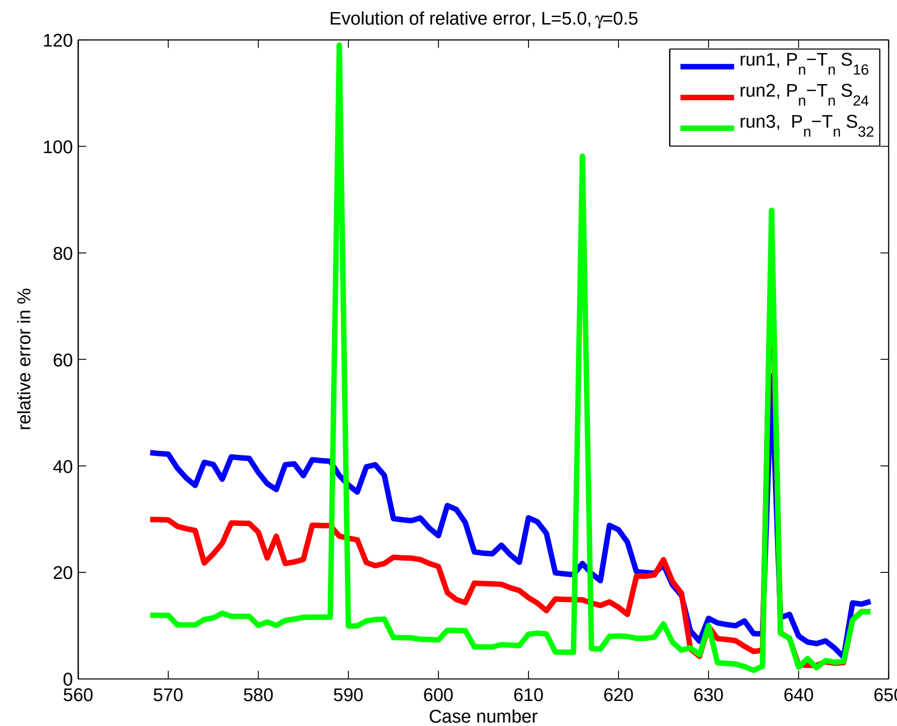


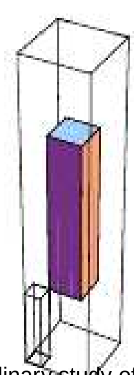




Results for L $= 5.0 \& \gamma = 0.5$







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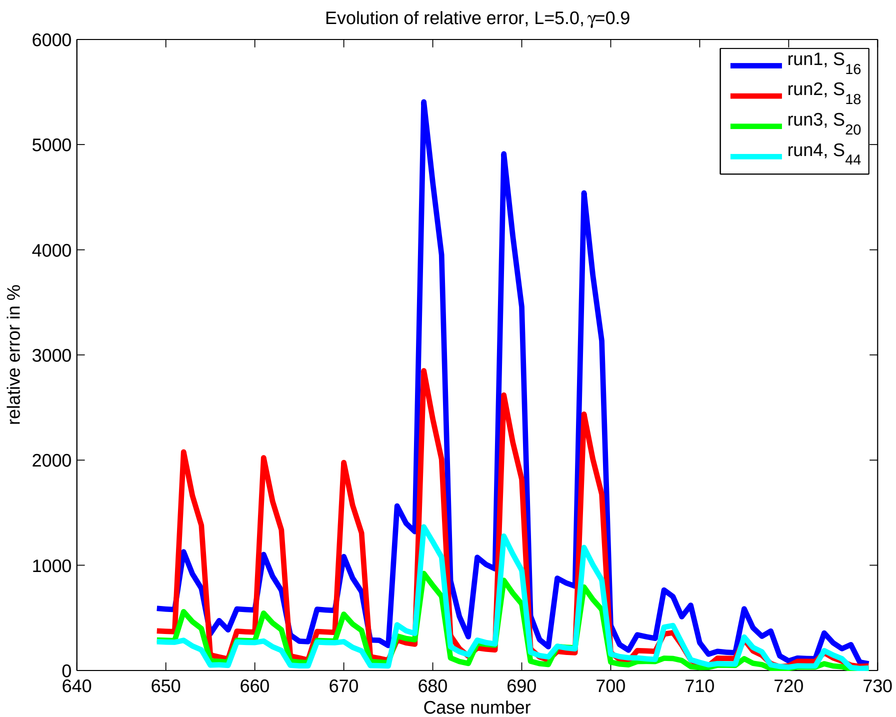
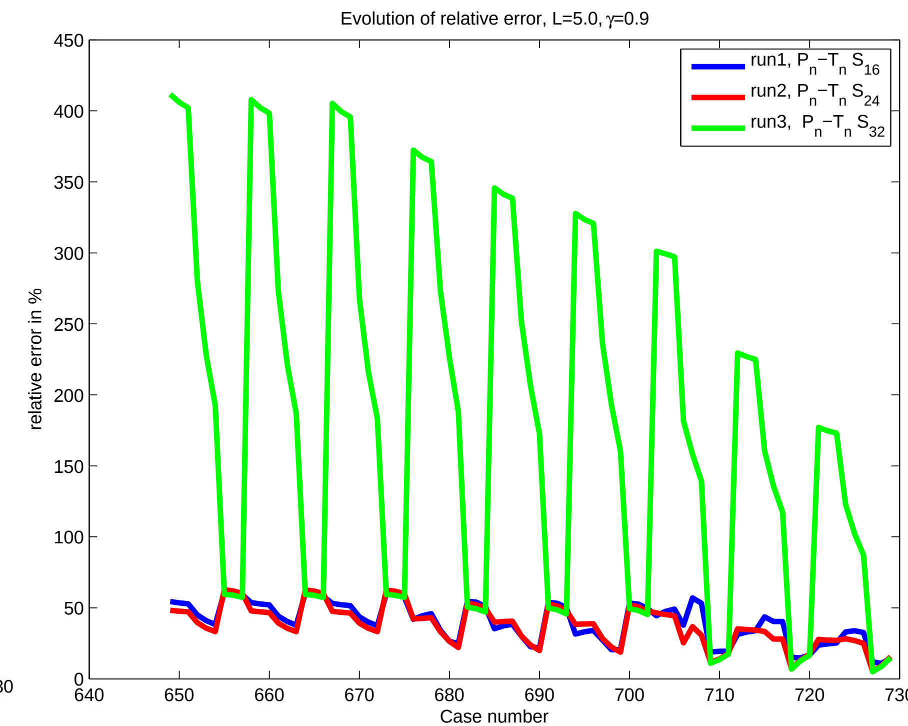
Results for $\mathrm{L} = 5.0 \& \gamma = 0.9$ 1





Conclusions

- General conclusion on this benchmark:
  - Computational challenge for a transport code (deterministic *and* Monte-Carlo).
  - Large amount of datas (15×729 numerical results) per run.
  - **Difficulty to get precise averaged flux value over a small volume, far from the source.**
  - Mean free path can reach a value of 25 cm.
- Need to obtain definitive reference solutions ($\sim$ 30 MCNP5 solutions still have important statistical errors).
- Require the use of *hybrid* calculation,*i.e.*, coupled deterministic-Monte Carlo.
- Final release planned for the beginning of 2009.

Conclusions

- Overview of the DRAGON results:
  - Confrontation to results of other deterministic codes such as TORT, PENTRAN and IDT(APOLLO2) are encouraging.
- S_N suffer deeply from the ray-effect: increase angular order can remedy.
- However, large amount of unknowns appear, due to DD discretization (i.e. ~ 32000000 for 333X3X cases with S_{54}).
- MOC far more expensive in term of CPU time than $\mathbf{S_N}$ (factor of 3)
- Improvements have already been made: quadruple range angular quadrature (QR_n) available up to order 74 in DRAGON.