Splitting methods with processing in path integral Monte Carlo simulations

Fernando Casas
www.gicas.uji.es

Departament de Matemàtiques
Institut de Matemàtiques i Aplicacions de Castelló (IMAC)
Universitat Jaume I
Castellón, Spain

7 September, 2010

Splitting for ODEs

- If f in
$$\dot{x} = f(x), \qquad x_0 = x(t_0) \in \mathbb{R}^D, \tag{1}$$
can be expressed as $f = f^{[a]} + f^{[b]}$, such tat
$$\dot{x} = f^{[a]}(x), \qquad \dot{x} = f^{[a]}(x), \qquad x_0 = x(t_0) \tag{2}$$
can be integrated exactly, with solutions $\varphi_h^{[a]}(x_0)$ and $\varphi_h^{[b]}(x_0)$ at $t = h$, then
$$\chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]} \tag{3}$$
is a first order approximation, $\chi_h(x_0) = x(h) + \mathcal{O}(h^2)$
- The composition
$$\mathcal{S}_h^{[2]} = \varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]} \tag{4}$$
furnishes a second-order numerical scheme (leapfrog, Strang, Störmer–Verlet, ...)

Splitting for ODEs

- Higher order approximations (order r):

$$\psi_h = \varphi_{ha_1}^{[a]} \circ \varphi_{hb_1}^{[b]} \circ \varphi_{ha_2}^{[a]} \circ \cdots \circ \varphi_{ha_p}^{[a]} \circ \varphi_{hb_p}^{[b]}. \tag{5}$$

  with appropriately chosen weights a_i, b_i so that $\psi_h(x_0) = x(h) + \mathcal{O}(h^{r+1})$
- The scheme is *symmetric* if $a_i = a_{p+1-i}$, $b_p = 0$ and $b_i = b_{p-i}$.
- By convention, method (5) has p stages
- Order conditions: polynomial equations to be satisfied by the parameters of the method so that approximates the exact solution up to $\mathcal{O}(h^r)$.

Processing

- First considered by J. Butcher in 1969 in the context of Runge–Kutta methods.
- Idea: to 'enhance' the integrator ψ_h by a change of variables given by a map π_h so that

$$\hat{\psi}_h = \pi_h \circ \psi_h \circ \pi_h^{-1} \tag{6}$$

  is of order higher than ψ_h.
- ψ_h is the kernel and π_h is the (post-)processor or corrector of the *processed* method $\hat{\psi}_h$.
- After n steps: $\hat{\psi}_h^n = \pi_h \circ \psi_h^n \circ \pi_h^{-1}$
- *Pre-processor* π_h^{-1} applied only once, then ψ_h acts once per step and finally π_h is evaluated only when output is required

Processing

- Advantageous if $\hat{\psi}_h$ is more accurate than ψ_h and the cost of π_h is negligible
- Since the mid-1990s, it has been used in geometric numerical integration (Sanz-Serna *et al.*, McLachlan, Wisdom, Suzuki, Blanes, Murua, Ros, C.,etc.).
- The method ψ_h is of *effective order* r if a post-processor π_h exists for which $\hat{\psi}_h$ is of (conventional) order r, that is,

$$\pi_h \circ \psi_h \circ \pi_h^{-1}(x_0) = x(h) + \mathcal{O}(h^{r+1}).$$

An example

- Leapfrog *is* a processed method

$$\begin{aligned} \mathcal{S}_h^{[2]} &= \varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]} = \varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_h^{[a]} \circ \varphi_{-h}^{[a]} \circ \varphi_{h/2}^{[a]} \\ &= \varphi_{h/2}^{[a]} \circ \chi_h \circ \varphi_{-h/2}^{[a]} = \pi_h \circ \chi_h \circ \pi_h^{-1}, \end{aligned} \tag{7}$$

  with $\pi_h = \varphi_{h/2}^{[a]}$.

- Hence, $\chi_h = \varphi_h^{[b]} \circ \varphi_h^{[a]}$ is of effective order 2.

Splitting methods with processing

- Processed methods whose kernel is an splitting method
- Several advantages:
  1. Many of the order conditions can be satisfied by using π_h
  2. The kernel has to verify a much reduced set of constraints with simpler structure
  3. It is possible to achieve high order with fewer stages
  4. The processor can be approximated in a cheap way
  5. For some problems the analysis of the kernel is particularly simple (e.g., linear problems)

Positive coefficients?

- When order $r \geq 3$, splitting methods (5) involve some negative coefficients
- They cannot be used for certain problems, e.g., ODEs defined in semigroups (G. Vilmart & P. Chartier talks)
- This result can be established as a theorem (Sheng, Suzuki). For an elementary proof, Blanes-C.
- Question: is this also true for processed methods?
- The theorem applies to the whole composition $\hat{\psi}_h = \pi_h \circ \psi_h \circ \pi_h^{-1}$, but may be ψ_h could involve only positive coefficients.
- The answer is no.

Positive coefficients?

- When order $r \geq 3$, splitting methods (5) involve some negative coefficients
- They cannot be used for certain problems, e.g., ODEs defined in semigroups (G. Vilmart & P. Chartier talks)
- This result can be established as a theorem (Sheng, Suzuki). For an elementary proof, Blanes-C.
- Question: is this also true for processed methods?
- The theorem applies to the whole composition $\hat{\psi}_h = \pi_h \circ \psi_h \circ \pi_h^{-1}$, but may be ψ_h could involve only positive coefficients.
- The answer is no.

Negative coefficients in the kernel

Theorem (Blanes-C, Chin 2005)

At least one of the a_i as well as one of the b_i coefficients have to be negative in the composition

$$\psi_h = \varphi^{[a]}_{ha_1} \circ \varphi^{[b]}_{hb_1} \circ \varphi^{[a]}_{ha_2} \circ \cdots \circ \varphi^{[a]}_{ha_p} \varphi^{[b]}_{hb_p}$$

if ψ_h is the kernel of a processed method of order (or equivalently if ψ_h is of effective order) $r \geq 3$.

- Thus the presence of negative coefficients in kernels of effective order $r \geq 3$ is unavoidable.
- Is it possible to circumvent this (fundamental) difficulty?

One (partial) remedy: 'modified potentials'

- For Hamiltonian systems $H(p,q) = \frac{1}{2} p^T \mathrm{M} p + V(q)$, then $f^{[a]} = \nabla T(p)$ and $f^{[b]} = \nabla V(q)$ and

$$\begin{aligned} \varphi_{ha}^{[a]}(x_0) &= (q_0 + h\, a\, \mathrm{M}^{-1}\, p_0,\, p_0)^T \\ \varphi_{hb}^{[b]}(x_0) &= (q_0,\, p_0 - h\, b\, \nabla V(q_0))^T. \end{aligned} \tag{8}$$

- If $\{f^{[a]}, f^{[b]}\}$ denotes the Poisson bracket, then

$$f^{[bab]} \equiv \{f^{[b]}, \{f^{[a]}, f^{[b]}\}\} = -(\nabla V)^T \mathrm{M}^{-1} \nabla V$$

  depends only on q
- Then $\{f^{[b]}, \{f^{[b]}, \{f^{[a]}, f^{[b]}\}\}\} = 0$, the flow corresponding to the 'potential' $f^{[bab]}$ is explicitly computable and can be included in the integrator

Examples of 'modified potentials'

- Alternatively, replace $\varphi_{hb_i}^{[b]}$ by $\varphi_{h;b_j,c_j}^{[b,c]}$, the flow corresponding to the 'modified potential'

$$W_{b_j,c_j} = b_j V(q) - c_j h^2 (\nabla V(q))^T \mathrm{M}^{-1} \nabla V(q).$$

- Order 4

$$\psi_h \quad = \quad \varphi_{h/6}^{[b]} \circ \varphi_{h/2}^{[a]} \circ \varphi_{h;2/3,1/72}^{[b,c]} \circ \varphi_{h/2}^{[a]} \circ \varphi_{h/6}^{[b]}$$

(Chin)

- Effective order 4

$$\psi_h \quad = \quad \varphi_{h/2}^{[a]} \circ \varphi_{h;1,1/24}^{[b,c]} \circ \varphi_{h/2}^{[a]}$$

(Takahashi-Imada, Rowland)

- If modified potentials of higher degree are considered, then it is possible to build methods of order 6 and higher with a_i, b_i positive (BIanes-C.-Ros), e.g. the flow of

$$f^{[d]} \equiv \{f^{[b]}, \{f^{[b]}, \{f^{[a]}, \{f^{[a]}, f^{[b]}\}\}\}\}$$

- Unfortunately, for some problems the computation of these high-degree modified potentials is not feasible.

Open question: Is it possible to construct methods of effective order 6 involving only the modified potential $W_{b_j,c_j} \equiv b_j\, V(q) + c_j\, h^2 (\nabla V(q))^T \nabla V(q)$ with all the a_i and b_i coefficients being positive?

- Currently, there are no known methods with these features.

Path Integral Monte Carlo (PIMC)

- In condensed matter physics, splitting methods with positive coefficients could be extremely useful in path integral Monte Carlo simulations
- All static and dynamical properties of a quantum system described by a Hamiltonian $\mathcal{H}$ in thermal equilibrium at temperature T can be obtained from the thermal density matrix

$$\rho = \mathrm{e}^{-\beta \mathcal{H}},$$

where $\beta = 1/(k_B T)$ and k_B is the Boltzmann constant.

PIMC

- Thus, expectation value for some operator $\hat{O}$ corresponding to a physical observable O:

$$\langle \hat{O} \rangle = Z^{-1} \operatorname{Tr}\left(\exp(-\beta \mathcal{H}) \hat{O} \right) = Z^{-1} \sum_n \langle n | \exp(-\beta \mathcal{H}) \hat{O} | n \rangle, \tag{9}$$

  where Z is the partition function

$$Z = \operatorname{Tr}\left(\mathrm{e}^{-\beta \mathcal{H}} \right) = \sum_n \langle n | \mathrm{e}^{-\beta \mathcal{H}} | n \rangle, \tag{10}$$

  and the states $|n\rangle$ form a complete, orthonormal basis set.
- Since the eigenvalues of the Hamiltonian $\mathcal{H}$ are not generally known, one tries to evaluate the traces in (9) and (10) without diagonalizing the Hamiltonian.
- This can be done with the Feynman path integral approach.

PIMC

Within this approach, in position representation,

- Density matrix: $\rho(\mathbf{R}, \mathbf{R}'; \beta) \equiv \langle \mathbf{R} | \mathrm{e}^{-\beta \mathcal{H}} | \mathbf{R}' \rangle$;
- $\mathbf{R} \equiv \{\mathbf{r}_1, \ldots, \mathbf{r}_N\}$ and the elements of $\rho(\mathbf{R}, \mathbf{R}'; \beta)$ are positive and can be interpreted as probabilities
- Partition function: $Z = \int d\mathbf{R} \, \langle \mathbf{R} | \mathrm{e}^{-\beta \mathcal{H}} | \mathbf{R} \rangle \equiv \int d\mathbf{R} \, \rho(\mathbf{R}, \mathbf{R}; \beta)$
- Procedure:
  - Factorize $\exp(-\beta \mathcal{H}) = (\exp(-\varepsilon \mathcal{H}))^M$ with $\varepsilon = \beta / M$ and a positive integer M (number of *beads*)
  - Approximate $\exp(-\varepsilon \mathcal{H})$ in practical applications

PIMC

- Then

$$\rho(\mathbf{R}_0, \mathbf{R}_M; \beta) = \int \cdots \int d\mathbf{R}_1 d\mathbf{R}_2 \cdots d\mathbf{R}_{M-1}\, \rho(\mathbf{R}_0, \mathbf{R}_1; \varepsilon) \times \rho(\mathbf{R}_1, \mathbf{R}_2; \varepsilon) \cdots \rho(\mathbf{R}_{M-1}, \mathbf{R}_M; \varepsilon). \quad (11)$$

- The goal is then to construct a sufficiently accurate approximation to the density matrix while minimizing the number of integrals involved in (11), i.e., the number of *beads* M
- Finally

$$Z = \int \cdots \int d\mathbf{R}_0 d\mathbf{R}_1 d\mathbf{R}_2 \cdots d\mathbf{R}_{M-1}\, \rho(\mathbf{R}_0, \mathbf{R}_1; \varepsilon) \times \rho(\mathbf{R}_1, \mathbf{R}_2; \varepsilon) \cdots \rho(\mathbf{R}_{M-1}, \mathbf{R}_0; \varepsilon), \quad (12)$$

PIMC

- Typically, $\mathcal{H} = \hat{K} + \hat{V}$: kinetic + potential energy

$$\hat{K} = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2$$

- Density matrix corresponding to $\hat{K}$ and $\hat{V}$ can be computed explicitly in position space.
- Approximate $\mathrm{e}^{-\varepsilon \mathcal{H}}$ by symmetric products of $\mathrm{e}^{-\varepsilon \hat{K}}$ and $\mathrm{e}^{-\varepsilon \hat{V}}$
- Simplest approximation (primitive action PA):

$$\mathrm{e}^{-\varepsilon(\hat{K}+\hat{V})} \simeq \mathrm{e}^{-\varepsilon \hat{K}}\, \mathrm{e}^{-\varepsilon \hat{V}}, \tag{13}$$

- In this case

$$\rho(\mathbf{R}_0, \mathbf{R}_2; \varepsilon) \approx \int d\mathbf{R}_1 \langle \mathbf{R}_0 | \mathrm{e}^{-\varepsilon \hat{K}} | \mathbf{R}_1 \rangle \langle \mathbf{R}_1 | \mathrm{e}^{-\varepsilon \hat{V}} | \mathbf{R}_2 \rangle.$$

- First order in $\varepsilon = \beta/M$ (effective order 2)

Higher order actions

- To study a fully quantum regime at very low temperatures, M increases very fast and the efficiency of the simulation suffers.
- Higher actions (higher order approximations in ε) are required.
- Symmetric factorizations of the form

$$\mathrm{e}^{h(\hat{K}+\hat{V})} \simeq \prod_{i=1}^{p} \mathrm{e}^{a_i h \hat{K}} \mathrm{e}^{b_i h \hat{V}}, \tag{14}$$

  where $h \equiv -\varepsilon$ and coefficients $\{a_i, b_i\}$ to be determined.
- *All these parameters must be positive*.
- Only in this way the integrand in Z can be normalized as a probability distribution and standard Metropolis Monte Carlo methods can be used

Higher order actions

- We must introduce modified potentials $\hat{W}_{b_i,c_i} = b_i \hat{V} + c_i h^2 [\hat{V}, [\hat{K}, \hat{V}]]$

Important feature: the trace in Z is invariant under similarity, so that we may construct only the kernel of a processed scheme to approximate $\mathrm{e}^{-\beta H}$ (*no processor is necessary*).

- The method $\psi_h = \mathrm{e}^{\frac{h}{2}\hat{K}} \mathrm{e}^{h\hat{W}_{1,1/24}} \mathrm{e}^{\frac{h}{2}\hat{K}}$ leads to Z accurate up to fourth order (Takahashi–Imada action).

Higher order actions

- Still more accuracy is necessary to deal properly with fully quantum fluids at ultra low temperature.
- Real fourth-order actions, possibly (hopefully!) of effective order 6.

It makes sense then to analyze whether it is possible to design methods of order four and effective order six containing only positive $\{a_i, b_i\}$ coefficients in the composition.

A particular method

- Recently, the 4th-order symmetric kernel (Scuro-Chin'05)

$$\psi_h = \mathrm{e}^{ha_1\hat{K}}\mathrm{e}^{h\hat{W}_{b_1,c_1}}\mathrm{e}^{ha_2\hat{K}}\mathrm{e}^{h\hat{W}_{b_2,c_2}}\mathrm{e}^{ha_2\hat{K}}\mathrm{e}^{h\hat{W}_{b_1,c_1}}\mathrm{e}^{ha_1\hat{K}}$$

  has been analyzed in quantum MC simulations (Sakkos-Casulleras-Boronat, 2009).

- Two free parameters: $0 \leq \alpha \leq \frac{1}{2}, \quad 0 \leq t_0 \leq \frac{3-\sqrt{3}}{6}$

$$\begin{aligned} a_1 &= t_0, & b_1 &= \frac{1}{6(1-2t_0)^2}, & c_1 &= u_0\,\alpha \\ a_2 &= \frac{1}{2} - t_0, & b_2 &= 1 - 2b_1, & c_2 &= u_0(1-2\alpha) \\ u_0 &= \frac{1}{12}\left(1 - \frac{1}{1-2t_0} + \frac{1}{6(1-2t_0)^3}\right) \end{aligned}$$

  so that all the a_i, b_i are positive.

Experimental conclusions

- The required M to reproduce the exact energy is much smaller than with PA and TIA (larger 'time steps' ε)
- Empirical procedure for adjusting α and t_0 to improve accuracy from 4th-order to 6th-order
- Error minimized with $\alpha = 0.33$ and $t_0 = 0.1215$. This is exact for the harmonic oscillator and remains approximately true for other systems (H_2 drop and liquid ^{4}He).
- Goals:
  - Explain these observed phenomena
  - Construct new schemes with better efficiency on an enlarged range of values of ε

Analysis of a family of 4th-order actions

- Ansatz: symmetric composition

$$\psi_h = \prod_{i=1}^{p} \exp(a_i h \hat{K}) \exp(h \hat{W}_{b_i,c_i})$$

- Order conditions (up to $r = 4$):

$$\sum_{i=1}^{p} a_i = 1, \qquad \sum_{i=1}^{p} b_i = 1, \qquad \sum_{i=1}^{p} b_i \left(\sum_{j=1}^{i} a_j \right)^2 = \frac{1}{3}$$

$$\frac{1}{2} \sum_{i=1}^{p} a_i \left(\sum_{j=i}^{p} b_j \right)^2 - \sum_{i=1}^{p} c_i = \frac{1}{6}$$

- Two more equations to achieve order 6:

$$G_1 \equiv 2\alpha_1 - \alpha_2 - \frac{1}{120} = 0, \qquad G_2 \equiv \alpha_3 + \alpha_4 - \frac{1}{60} = 0$$

- α_1, α_2: polynomials in terms of a_i, b_i
- α_3, α_4 depending linearly on c_i.
- The analysis is simpler in terms of

$$s_i \equiv \sum_{j=1}^{i} a_j, \qquad s_0 \equiv 0, \qquad s_p = 1,$$

- Two types of symmetric compositions:
  - ABA-composition: $b_p = 0, \quad b_{p-i} = b_i, \quad s_{p-i} = 1 - s_i.$
  - BAB-composition: $b_{p+1-i} = b_i, \quad s_{p-i} = 1 - s_{i+1}$
- a_i are non-negative as long as $s_0 = 0 \leq s_1 \leq s_2 \leq \cdots \leq s_p = 1$

ABA-compositions

- $p = 4$ is the minimum number of stages:

$$\psi_h = \mathrm{e}^{ha_1 K} \mathrm{e}^{hW_{b_1,c_1}} \mathrm{e}^{ha_2 K} \mathrm{e}^{hW_{b_2,c_2}} \mathrm{e}^{ha_2 K} \mathrm{e}^{hW_{b_1,c_1}} \mathrm{e}^{ha_1 K}$$

- Three solutions for b_1, b_2 and s_1, but only one real: $s_1 \simeq 0.486421$. All a_i coefficients positive, but $b_1 = 225.975$, $b_2 = -450.949$.
- At least one b_j negative.

ABA $p = 4$

- When $\hat{V} = \frac{1}{2}\lambda^2 x^2$, it *is* possible to get ABA methods with $p = 4$ of order 4 and effective order 6: if

$$t_0 = s_1 \in (0,\, 0.132024) \cup (0.142326, 0.180679)$$

  then all the coefficients are positive and the schemes are of effective order 6 for the harmonic oscillator.
- For $s_1 = t_0 = 0.1215$, one gets $\alpha = 0.329556$.
- This explains the observed behavior
- *The composition is no longer of effective order 6 for a general potential*
- Identical conclusions are derived for $p = 5$ and $p = 6$.

BAB methods

- Here also $p = 4$:

$$\psi_h = \mathrm{e}^{h\hat{W}_{b_1,c_1}}\mathrm{e}^{ha_1\hat{K}}\mathrm{e}^{h\hat{W}_{b_2,c_2}}\mathrm{e}^{ha_2\hat{K}}\mathrm{e}^{h\hat{W}_{b_2,c_2}}\mathrm{e}^{ha_1\hat{K}}\mathrm{e}^{h\hat{W}_{b_1,c_1}}. \quad (15)$$

- FSAL property: 3 stages (same as before)
- 3 variables to analyze: $b_1, b_2, a_1 = s_2$
- All coefficients are positive when $s_2 \in (0.211325, 0.350226) \cup (0.459992, 0.5)$ for the harmonic oscillator
- No longer true for a general potential
- Same behavior for $p \geq 5$.

Linear stability

- In addition to order of accuracy, stability
- Stable numerical integrator: the numerical solution does not tend to infinity when the exact solution is bounded
- Numerical integrators with a large stability interval are very convenient in PIMC: in this way h is as large as possible, M is small and the computational complexity is reduced
- Linear stability is easy to analyze for splitting methods
- They are applied to the 1-dimensional harmonic oscillator

$$y'' + \lambda^2 y = 0, \qquad \lambda > 0,$$

with $x = (q,p)^T = (q,p) = (\lambda y, y')^T$

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \Big[\underbrace{\begin{pmatrix} 0 & \lambda \\ 0 & 0 \end{pmatrix}}_{A} + \underbrace{\begin{pmatrix} 0 & 0 \\ -\lambda & 0 \end{pmatrix}}_{B} \Big] \begin{pmatrix} q \\ p \end{pmatrix},$$

Linear stability

- Exact solution:

$$O(x) = \begin{pmatrix} \cos x & \sin x \\ -\sin x & \cos x \end{pmatrix}, \qquad x = h\lambda,$$

- Approximation:

$$\begin{aligned} K(x) &= \begin{pmatrix} 1 & a_1 x \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -x(b_1 - 2c_1 x^2) & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & a_p x \\ 0 & 1 \end{pmatrix} \\ &\quad \times \begin{pmatrix} 1 & 0 \\ -x(b_p - 2c_p x^2) & 1 \end{pmatrix} \\ &= \mathrm{e}^{h a_1 \hat{K}} \, \mathrm{e}^{h \hat{W}_{b_1, c_1}} \cdots \mathrm{e}^{h a_p \hat{K}} \, \mathrm{e}^{h \hat{W}_{b_p, c_p}}. \end{aligned}$$

- Goal: find the maximal value of x for which $K(x)^n$ remain bounded for all n

- Stability threshold: the largest non-negative real number such that $K(x)$ is stable for all $x \in (-x_*, x_*)$
- $K(x)^n$ can be bounded independently of $n \geq 1$ for $x \in (-x_*, x_*)$ if all the eigenvalues of K lie on the stability interval $(-x_*, x_*)$.
- $x_* \leq 2p$ since $2p$ is the maximal value of the stability threshold, which is achieved by the concatenation of p steps of length h/p of the leapfrog scheme
- For processed methods the linear stability is determined only by the kernel

- We analyze the linear stability of the 1-parameter 4th-order actions considered before
- Procedure: to determine for each family the stability threshold x_* as a function of the free parameter and select the parameter leading to the largest value of x_*.
- Results:

Method	Parameter	Largest x_*	x_*/p
ABA	$s_1 = 0.1234$	3.0731	1.02436
BAB	$s_2 = 0.2785$	3.1399	1.04663

- x_*/p should be compared with 2, the maximal stability threshold attained by leapfrog

Remarks

- With the BAB composition it is possible to achieve a larger stability interval: new method which can be used with a larger step size
- For the value considered by Boronat *et al.* for ABA, $s_1 = t_0 = 0.1215$, one has $x_*/p = 1.02419$
- It is possible to adjust the parameter to get higher stability

Conclusions:

- We have provided a theoretical justification of previous empirical observations
- We have designed new methods within this family with the same computational cost and better properties (larger time steps)
- It is not strictly necessary to satisfy exactly all the effective order conditions at order 6, only in the linear case
- Important: to have a large stability threshold
- Essential: positive coefficients

Outlook:

- Design new methods with more stages than strictly necessary (e.g., $p = 5$ or $p = 6$) and use the extra parameters to fulfill effective order conditions at higher orders for the linear case, whereas
  - keeping all the coefficients positive
  - ensuring a large stability interval
- Apply the new methods in actual Monte Carlo simulations