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Solve-operator algorithms in high-precision simulators of complex systems

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Алгоритми розв’язуючих операторів у чисельному моделюванні складних систем з підвищеною точністю

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Using solve-operator methods we develop high-precision numerical simulators of graph-operator models made up on basis of their local sub-models approximations by systems of deterministic differential equations with random value parameters on optimized time intervals.

Key Words: solve-operators, complex systems, numerical algorithms for high order accuracy, Cauchy problem.

За допомогою методів розв’язуючих операторів будуються алгоритми обчислення з підвищеною точністю траєкторій граф-операторних моделей із локальними підсистемами, що апроксимуються системами диференціальних рівнянь із випадковими значеннями параметрів на оптимізованих інтервалах часу.

Ключові слова: розв’язуючі оператори, складні системи, числові алгоритми високого порядку точності, задача Коші.

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We consider a complex system

$$A(x,u,q,\theta) \square \left(A_1(x,u,q,\theta),\dots,A_{N_k}(x,u,q,\theta)\right)=0$$

$$A_k(x,u,q,\theta) \square (A_{k1}(x_{k1},z_{k1},u_{k1},q_{k1},\theta_{k1}),\dots,$$
$$A_{kN_{ks}}(x_{kN_{ks}},z_{kN_{ks}},u_{kN_{ks}},q_{kN_{ks}},\theta_{kN_{ks}})),$$
$$(x,u,q,\theta) \square \{(x_k,u_k,q_k,\theta_k)\}_{k=1}^{N_k},\ (x_k,u_k,q_k,\theta_k) \square$$
$$\square \{(x_{ks},u_{ks},q_{ks},\theta_{ks})\}_{s=1}^{N_{ks}}$$

of sub-models $A_{ks}(x_{ks},z_{ks},u_{ks},q_{ks},\theta_{ks})=0$, $k=\overline{1,N_k}$, $s=\overline{1,N_{ks}}$ modeling interdependences between subsystem’s states x_{ks}, parameters q_{ks}, random values θ_{ks}, controls u_{ks}, and influences z_{ks}, $z_{ks}=\varphi_{ks}(x,u,q,\theta)$ of others subsystems. ET-adequate simulators of dynamical systems are defined by restrictions on admissible simulation errors *E*(*p*) of the trajectory x_{ks} simulation (calculation) under restrictions on computational burden (time extended) *T*(*p*) required to calculate the trajectory x_{ks} using a simulator with parameters p. The optimized values of p are defined as minimizers of the criteria *J*(*p*)=*KT*(*p*)+*E*(*p*) on selected parameterized sets of simulators (based on mathematical models with varied aggregation levels, resolving power, and information sources). The subsystems optimization realizes by iterative procedures of detecting those of the subsystems that have be decomposed and those that have to be aggregated. Thus simulator optimization procedures have to detect those of too complicated subsystem’s that have to be replaced by simplified models aiming to decrease *T*(*p*) without particular increasing of the overall error *E*(*p*). In this way to simulate trajectories $x_{ks}(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})$ of the complex stochastic subsystem $A_{ks}(x_{ks}, z_{ks}, u_{ks}, q_{ks}, \theta_{ks}) = 0$ they perform successful approximations by simple stochastic differential equation subsystems (SDE)

$$dx(t) = a(x(t), u, q, \theta)dt + b(x(t), u, q, \theta)dw(t),$$
$$x(t) \in R^n,\ a(\cdot) = \{a_i(\cdot), i = \overline{1..n}\},$$
$$b(\cdot) = \{b_{ij}(\cdot), i = \overline{1..n}, i = \overline{1..m}\},$$

with probability densities $p \equiv p(x, t \mid x_0, t_0, u, q, \theta)$ calculated by the Fokker-Planck equation

$$\frac{\partial p(x,t)}{\partial t} = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i}[a_i(x(t), u, q, \theta)\, p(x,t)] + $$
$$+\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial^2}{\partial x_i \partial x_j}[\overline{b}_{ij}(x(t), u, q, \theta)\, p(x,t)].$$

For the trajectory $x_{ks}(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})$ approximation they use the Euler-Maruyama simulator

$$x(t_{i+1}) = x(t_i) + a(x(t_i), u, q, \theta)(t_{i+1} - t_i) +$$
$$+b(x(t_i), u, q, \theta)(w(t_{i+1}) - w(t_i))$$

or the more accurate Milstein simulator

$$x(t_{i+1}) = x(t_i) + a(x(t_i), u, q, \theta)(t_{i+1} - t_i) +$$
$$+b(x(t_i), u, q, \theta)(w(t_{i+1}) - w(t_i)) +$$
$$+\frac{1}{2} b(x(t_i), u, q, \theta) b^T(x(t_i), u, q, \theta)((w(t_{i+1}) -$$
$$-w(t_i))^2 + t_i - t_{i+1}).$$

As well simulators of $\tilde{\tilde{f}}(t, x(t))$ are based on the Ito formula

$$d\tilde{\tilde{f}}(t, x(t)) = [\partial_t \tilde{\tilde{f}}(t, x(t)) +$$
$$+a(x(t), u, q, \theta)\partial_x \tilde{\tilde{f}}(t, x(t))dt +$$
$$+0{,}5 b^2(x(t), u, q, \theta)\partial_{xx}^2 \tilde{\tilde{f}}(t, x(t))]dt +$$
$$+b(x(t), u, q, \theta)\partial_x \tilde{\tilde{f}}(t, x(t))dw(t).$$

In cases of the simplified sub-models:

$$dx_{ks}^1(t) = a_{ks}^1(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})dt +$$
$$+b_{ks}^1(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})dw(t),$$
$$dx_{ks}^2(t) = x_{ks}^2(t)(a_{ks}^2(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})dt +$$
$$+b_{ks}^2(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})dw(t)),$$
$$dx_{ks}^3(t) = a_{ks}^3(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})x_{ks}^3(t)dt +$$
$$+b_{ks}^3(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})dw(t),$$
$$dx_{ks}^4(t) = (A(u(t), q(t), \theta(t), t)x_{ks}^4(t) +$$
$$+c(u(t), q(t), \theta(t), t))dt + B(u(t), q(t), \theta(t), t)dw(t)$$

with Brownian movements $w(t) \equiv (w_1(t), ..., w_m(t))$,

$$dw_i(t) \equiv w_i(t+dt) - w_i(t),\ \ E(dw_i^2(t)) = \sigma_i^2 dt,$$
$$E(dw_i(t)dw_j(t)) = 0,\ i \neq j$$

simulators are given by simple formulae:

$$x_{ks}^1(t) = x_{ks}^1(t_0) + a_{ks}^1(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})(t - t_0) +$$
$$+b_{ks}^1(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})w(t - t_0),$$
$$x_{ks}^2(t) = \exp((a_{ks}^2(u_{ks}, q_{ks}, \theta_{ks}, z_{ks}) -$$
$$-(b_{ks}^2)^2(u_{ks}, q_{ks}, \theta_{ks}, z_{ks}) / 2)(t - t_0) +$$
$$+b_{ks}^2(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})w(t - t_0)),$$
$$x_{ks}^3(t) = x_{ks}^3(t_0)\exp(a_{ks}^3(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})(t - t_0)) +$$
$$+b_{ks}^3(u_{ks}, q_{ks}, \theta_{ks}, z_{ks}) \times$$
$$\times \int_{t_0}^{t} \exp(a_{ks}^3(u_{ks}, q_{ks}, \theta_{ks}, z_{ks})(t - \tau))dw(\tau),$$
$$x_{ks}^4(t) = \Phi(t)x_{ks}^4(t_0) +$$
$$+\Phi(t)\int_{t_0}^{t} \Psi(\tau)(c(u(\tau), q(\tau), \theta(t), \tau) +$$
$$B(u(\tau), q(\tau), \theta(\tau), \tau)dw(\tau),$$

with the fundamental matrices $\Phi(\cdot)$ and $\Psi(\cdot)$ of associated homogeneous linear system and it's conjugate system.

In case of general stochastic subsystems the simplified simulators of the trajectories $x_{ki}(t, u_{ki}, q_{ki}, \theta_{ki})$ with given sets of the control functions u_{ki}, random values $\theta_{ki} \in \mathbb{R}^{n_{ki}}$ and with given sets Q_{ki} of unknown admissible values of parameters q_{ki}, we design by simplified systems

$$t_0 = \overline{t}(u_{k0}, q_{k0}, \theta_{k0}) \in R,$$
$$x_{k0}(t_0) = \overline{x}_{k0}(t_0, u_{k0}, q_{k0}, \theta_{k0}) \in R^{n_{kx}},$$
$$dx_{ki}(t) = a_{ki}(x_{ki}(t), u_{ki}, q_{ki}, \theta_{ki}, t, \omega_{ki}(x_{ki}(t_i), t_i, q_{ki}, \theta_{ksi}, t))dt,$$
$$t \in [t_i, t_{i+1}],$$
$$t_{i+1} = \tau(x_{k(i-1)}(t_i), t_i, u_{ki}, q_{ki}, \theta_{ki}, z_{ki}) > t_i,$$

$$x_{k(i+1)}(t_{i+1}) = \psi(x_{ki}(t_{i+1}), t_{i+1}, u_{k(i+1)}, \theta_{k(i+1)}, z_{k(i+1)})$$

with optimized distribution functions

$$\tilde{F}_{ki}(\tilde{\theta}_{ki} \mid (x_{k(i-1)}(t_i), t_i, q_{k(i-1)}, \theta_{k(i-1)}, z_{k(i-1)}).$$

To design high precision solve-operator methods of calculating $x_{ksi}(t,\overline{p},\overline{q},\overline{\theta})$ with given $\overline{q}$, $\overline{u}$ and $\overline{\theta}$ we implement the asymptotic solve operator [1]

$$\overline{x}(t+h) = p(t+h) + \\ + \int_t^{t+h} Q(\tau)\Big(a(p(\tau),\overline{u},\overline{q},\overline{\theta},\tau,\omega(x(t_i),t_i,\overline{u},\overline{q},\overline{\theta},\tau)) - . \\ - dp(\tau)/d\tau\Big)d\tau.$$

It was proved that the asymptotic equalities

$$p(\tau) = x(\tau) + O(h^l), \\ dQ(\tau)/d\tau = O(h^k) - \\ -Q(\tau)a'_x(p(\tau),\overline{u},\overline{q},\overline{\theta},\tau,\omega(x(t_i),t_i,\overline{u},\overline{q},\overline{\theta},\tau)), \\ Q(t+h) = I.$$

Imply the high precision asymptotic equality

$$\overline{x}(t+h) = x(t+h) + O(h^s),\ s=k+l+1,$$

in the neighborhood of the solution $x = x(\tau) \equiv x(\tau,\overline{u},\overline{q},\overline{\theta})$ of the system

$$dx(\tau)/d\tau = a(p(\tau),\overline{u},\overline{q},\overline{\theta},\tau,\omega(x(t_i),t_i,\overline{u},\overline{q},\overline{\theta},\tau)), \\ \tau \in (t,t+h) \subset [t_i,t_{i+1}].$$

The proposed high order simulators of the asymptotic solve operator

$$x(t+mh) = \\ = \int_t^{t+mh} \big[E - (\tau - t - mh) f'_x\big(p(t+mh),t+mh\big)\big] \times \\ \times \big[f\big(p(\tau),\tau\big) - \dot{p}(\tau)\big]d\tau + p(t+mh)$$

to be used on the time intervals $t \in [t_i,t_{i+1}]$ are defined by the approximations $p(\tau)$ of the system

$$\dot{x}(t) = f\big(x(t),t\big) \equiv \\ \equiv a_{ki}(x_{ki}(t),u_{ki},q_{ki},\theta_{ki},t,\omega_{ki}(x_{ki}(t_i),t_i,q_{ki},\theta_{ksi},t)), \\ x(t_0) = x^0 \in R^{n_1},\ n_1 \ge 1,\ t \ge t_0,$$

with the approximation error

$$\|x(\tau) - p(\tau)\| = O(h^s), \qquad \tau \in [t,t+mh],$$

giving the simulators error $O(h^{s+2})$.

Using the function notations

$$\theta(\tau;m) = f'_x\big(p(t+mh),t+mh\big) \times \\ \times \big[E - (\tau - t - mh)\big]\big[f\big(p(\tau),\tau\big) - \dot{p}(\tau)\big], \\ L_k(\tau) = a_1\tau^k + a_2\tau^{k-1} + \ldots + a_k\tau + a_{k+1}$$

we find the function $x(\tau)$ with bounded $x^{(r+1)}(\tau)$ on the interval $[t-mh,t+mh]$

$$x(\tau) = x(t) + (\tau - t)x'(t) + \frac{1}{2!}(\tau-t)^2 x''(t) + \ldots \\ + \frac{1}{r!}(\tau-t)^r x^{(r)}(t) + O(h^{r+1}).$$

Thus, the function

$$p(\tau) = x(t) + (\tau - t)x'(t) + \frac{1}{2!}(\tau-t)^2 x''(t) + \ldots \\ + \frac{1}{r!}(\tau-t)^r x^{(r)}(t),$$

approximates $x(t)$ on the interval $[t-mh,t+mh]$ with the error $O(h^{r+1})$.

Taking on the interval $[t,t+h]$ the approximation

$$p(\tau) = x(t) + (\tau - t)x'(t) + \frac{1}{2!}(\tau-t)^2 x''(t)$$

with the error $O(h^3)$ we obtain the simplified simulator

$$x(t+h) = p(t+h) + \int_t^{t+h} \theta(\tau;1)d\tau,$$

with $p(t+h)$ calculated by

$$p(t+h) = x(t) + hf\big(x(t),t\big) + \frac{h^2}{2}x''(t). \quad (1)$$

To calculate $\int_t^{t+h} \theta(\tau;1)d\tau$ by the approximated value $\int_t^{t+h} L_3(\tau)d\tau$ we calculate the solution $a_i,\ i=1,\ldots,4,$ of the system

$$\begin{cases} a_1t^3 + a_2t^2 + a_3t + a_4 = \theta(t;1) = 0, \\ a_1(t+h)^3 + a_2(t+h)^2 + a_3(t+h) + a_4 = \theta(t+h;1), \\ 3a_1t^2 + 2a_2t + a_3 = \dot{\theta}(t;1), \\ 3a_1(t+h)^2 + 2a_2(t+h) + a_3 = \dot{\theta}(t+h;1) \end{cases}$$

to obtain

$$\int_t^{t+h} L_3(\tau)d\tau = \left(\frac{1}{4}a_1\tau^4 + \frac{1}{3}a_2\tau^3 + \frac{1}{2}a_3\tau^2 + a_4\tau\right)\Bigg|_t^{t+h} = \frac{h}{12}\left(6\theta(t+h;1) - h\dot{\theta}(t+h;1)\right),$$

$$\int_t^{t+h} \theta(\tau;1)d\tau = \frac{h}{12}\left[6\theta(t+h;1) - h\dot{\theta}(t+h;1)\right] + O(h^5),$$

$$\begin{aligned} x(t+h) = x(t) + \frac{h}{12}\Big\{&6f\left(x(t),t\right) + 6f\left(p(t+h),t+h\right) - h\Big[\dot{f}\left(p(t+h),t+h\right) - \\ &-x''(t) + f'_x\left(p(t+h),t+h\right)\times \\ &\times\left[2f\left(x(t),t\right) - f\left(p(t+h),t+h\right) + 2hx''(t)\right]\Big]\Big\}. \end{aligned} \tag{2}$$

To simplify the calculation of the values of the function f at the points $\left(x(t_{k-1}+h), t_{k-1}+h\right)$ we implement the formula

$$\begin{aligned} f\left(x(t_{k-1}+h), t_{k-1}+h\right) = f\left(p(t_{k-1}+h), t_{k-1}+h\right) + \\ + f'_x\left(p(t_{k-1}+h), t_{k-1}+h\right)\left[x(t_{k-1}+h) - p(t_{k-1}+h)\right]. \end{aligned} \tag{3}$$

Here are results of calculation for oscillating systems

$$\begin{cases} \dot{x}_1(t) = -10x_2(t)/(t-10)^2, \ x_1(0) = 0, \\ \dot{x}_2(t) = 10x_1(t)/(t-10)^2, \ x_2(0) = 1 \end{cases}$$

with integration step $h = 0.1$.

Table 1

Absolute coordinate deviations from the analytical approximate solutions.

t	Runge-Kutta 4^{th} order accuracy method	Iteration formula (2)	Iteration formula (2) with regard (3)	Iteration formula (1)
0.1	2.41E-11 3.15E-14	3.54E-11 1.00E-13	3.54E-11 1.00E-13	8.38E-07 1.02E-06
0.5	1.74E-10 9.87E-13	2.06E-10 8.00E-12	2.06E-10 8.00E-12	9.17E-07 1.28E-06
3.0	2.17E-09 1.01E-09	4.15E-09 1.80E-09	4.15E-09 1.80E-09	1.74E-07 6.24E-06
7.0	8.67E-07 9.44E-07	1.06E-06 1.32E-06	1.06E-06 1.32E-06	2.29E-04 2.94E-04
8.5	1.69E-04 2.61E-04	2.25E-04 3.05E-04	2.25E-04 3.05E-04	2.81E-03 1.34E-02
9.0	3.82E-03 8.98E-03	4.87E-03 1.01E-02	4.87E-03 1.01E-02	1.95E-02 1.15E-01

From the approximation

$$x(\tau) = x(t) + (\tau-t)x'(t) + \frac{(\tau-t)^2}{2!}x''(t) + \frac{(\tau-t)^3}{3!}x'''(t) + O(h^4), \quad \tau\in[t,t+2h],$$

$$x'''(t) = \left(x''(t+h) - x''(t)\right)/h + O(h)$$

it follows that on the interval $[t, t+2h]$ the function

$$p(\tau) = x(t) + (\tau-t)x'(t) + \frac{(\tau-t)^2}{2}\left[1 - \frac{\tau-t}{3h}\right]x''(t) + \frac{(\tau-t)^3}{6h}x''(t+h),$$

approximates x with the error value of $O(h^4)$. Thus with $m = 2$ and

$$p(t+2h)=$$
$$= x(t)+2hf\left(x(t),t\right)+\frac{2}{3}h^2x''(t)+\frac{4}{3}h^2x''(t+h) \quad (4)$$

we have

$$x(t+2h)=p(t+2h)+\int_t^{t+2h}\theta(\tau;2)d\tau .$$

The approximated value of $\int_t^{t+2h}\theta(\tau;2)d\tau$ may be calculated by

$$\int_t^{t+2h}L_4(\tau)d\tau=$$
$$=\frac{h}{15}\left(16\theta(t+h;2)+7\theta(t+2h;2)-h\dot\theta(t+2h;2)\right),$$

giving

$$\int_t^{t+2h}L_4(\tau)d\tau=$$
$$=\left(\frac{1}{5}a_1\tau^5+\frac{1}{4}a_2\tau^4+\frac{1}{3}a_3\tau^3+\frac{1}{2}a_4\tau^2+a_5\tau\right)\Bigg|_t^{t+2h}$$

$$\begin{cases} a_1t^4+a_2t^3+a_3t^2+a_4t+a_5=\theta(t;2)=0,\\ a_1(t+h)^4+a_2(t+h)^3+a_3(t+h)^2+a_4(t+h)+a_5=\\ \qquad =\theta(t+h;2),\\ a_1(t+2h)^4+a_2(t+2h)^3+a_3(t+2h)^2+a_4(t+2h)+\\ \qquad +a_5=\theta(t+2h;2),\\ 4a_1t^3+3a_2t^2+2a_3t+a_4=\dot\theta(t;2)=0,\\ 4a_1(t+2h)^3+3a_2(t+2h)^2+2a_3(t+2h)+a_4=\\ \qquad =\dot\theta(t+2h;2). \end{cases}$$

From the formula

$$\int_a^b\varphi(\tau)d\tau=\frac{b-a}{90}\left(12\varphi\left(\frac{a+b}{2}\right)+32\left(\varphi\left(\frac{3a+b}{4}\right)+\right.\right.$$
$$\left.\left.+\varphi\left(\frac{a+3b}{4}\right)\right)+7\left(\varphi(a)+\varphi(b)\right)\right)-$$
$$-\frac{1}{1935360}(b-a)^7\varphi^{(6)}(\varsigma),\ \varsigma\in[a,b],$$

it follows

$$\int_t^{t+2h}\theta(\tau;2)d\tau=O(h^7)+$$
$$+\frac{h}{15}\left[16\theta(t+2h;2)+7\theta(t+2h;2)-h\dot\theta(t+2h;2)\right].$$

giving the high order simulators

$$f\left(p(t_{k-1}+h),t_{k-1}+h\right)=f\left(x(t_{k-1}+h),t_{k-1}+h\right)+$$
$$+f_x'\left(x(t_{k-1}+h),t_{k-1}+h\right)\left[p(t_{k-1}+h)-x(t_{k-1}+h)\right], \quad (5)$$

$$f\left(x(t_{k-1}+2h),t_{k-1}+2h\right)=f\left(p(t_{k-1}+2h),t_{k-1}+2h\right)+$$
$$+f_x'\left(p(t_{k-1}+2h),t_{k-1}+2h\right)\left[x(t_{k-1}+2h)-p(t_{k-1}+2h)\right], \quad (6)$$

$$x(t+2h)=p(t+2h)+$$
$$+\frac{h}{12}\Big\{-23f\left(x(t),t\right)+16f\left(p(t+h),t+h\right)+$$
$$+7f\left(p(t+2h),t+2h\right)+$$
$$+h\left[-9x''(t)-20x''(t+h)-\dot f\left(p(t+2h),t+2h\right)\right]+ \quad (7)$$
$$+hf_x'\left(p(t+2h),t+2h\right)\Big[-18f\left(x(t),t\right)+$$
$$+16f\left(p(t+h),t+h\right)+f\left(p(t+2h),t+2h\right)-$$
$$-h\left(8x''(t)+12x''(t+h)\right)\Big]\Big\},$$

on the intervals $t\in[t_i,t_{i+1}]$.

Table 2

Absolute coordinate deviations from the analytical approximate solutions.

t	Iteration formula (7)	Iteration formula (7) with regard (5), (6)	Iteration formula (4)
0.2	2.75E-12 2.80E-12	2.75E-12 2.80E-12	1.00E-10 1.03E-09
0.5	6.93E-12 6.50E-12	6.93E-12 6.50E-12	1.00E-10 1.27E-09
3.0	3.52E-10 1.02E-10	3.52E-10 1.02E-10	7.55E-09 7.38E-09
7.0	2.14E-07 5.11E-07	2.14E-07 5.11E-07	2.52E-06 4.48E-06
8.5	2.29E-04 3.14E-04	2.29E-04 3.14E-04	1.09E-03 3.74E-04
9.0	7.89E-03 1.98E-02	7.89E-03 1.98E-02	3.14E-02 3.30E-03

Conclusion

The proposed numerical algorithms based on methods of solve operators, enable to raise to high precision of the numerical simulators by implementation of high order asymptotic solve operators.

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