A new algorithm for solving differential equations - (session: Novel Algorithms for Bioinformatics)

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In some previous meetings of GCB (Bioinformatic Cooperation Group) we have reported about the progress in developing our new algorithm for the numerical integration of large stiff systems of ordinary differential equations (ODE).
The algorithm has a wide utilisation spectrum, including for example the simulation of signal pathways and large metabolic networks (neglecting spatial aspects such as transport and diffusion) in projects involving the virtual cell.
Our method is based on a new approach to the computation of a matrix exponential, includes an automatic correction of rounding errors, is not too expensive computationally, and lends itself to a short and robust software implementation that can be easily inserted in large simulation packages.
The algorithm is largely independent from ill-conditioning and is suitable for any nonlinear problem; moreover, being exact for linear problems, it is especially precise for quasi-linear problems, the most frequent kind in the real world.
The final version of the algorithm is just being published [1]. A preliminary numerical verification has been performed. The paper includes the encouraging results obtained on two sample problems.
The full C listing (including a sample problem) is available as free software, see [1].
Here we describe the main features of the algorithm. The main formulas are reported in fig. 1. Full details can be found in [1].

[1] Aluffi-Pentini F, De Fonzo V, Parisi V. A novel algorithm for the numerical integration of systems of ordinary differential equations arising in chemical problems. J. Math. Chem. In press.