PARTICULARS: EFFICIENT EVANS FUNCTION CALCULATIONS VIA NEUMANN AND MAGNUS EXPANSIONS

Summary, significance and objectives. A practical problem when integrating systems of linear ordinary differential equations, is that if we wish to sample the solution for a different value of an inherent parameter, then we must re-integrate. This is particularly inefficient when we want to accurately sample the solution over a continuous widespread set of parameter values. Though continuity methods resolve this issue locally, they still involve some degree of re-integration. A particular application we have in mind is that of evaluating the Evans function for different values of the spectral parameter, which involves repeated integration of the spectral equations. In this project we propose to extensively study a set of new efficient numerical methods based on Neumann and Magnus expansions, that completely avoid the need for re-integration. These methods were recently proposed by Aparicio, Malham & Oliver (2002); they extend and generalize work by Moan (1998). The basic idea is that we expand either the Neumann or Magnus series solution for such systems as a power series in the parameter(s) in question. The coefficients of the series can be precomputed to any required accuracy. Then we evaluate the series for any of the parameter values we wish to sample. This proposal is intended to crystallize and then implement these ideas. The realization of these methods will revolutionize Evans function calculations and the direct construction of the pure-point spectrum of linear operators. Our objectives are:

(1) Full error analysis of newly proposed Neumann and Magnus-based integrators for efficient parameter sampling of solutions of systems of linear ordinary differential equations. We will implement optimized time-step control and adaptivity.
(2) Qualitative and quantitative comparison with existing numerical schemes. In particular, variable time-step methods based on the Magnus expansion retain Lie group structure, which will be significant in Evans function calculations.
(3) Application of the numerical algorithms to constructing the Evans function for unstable pulse solutions in the Gray-Scott model. Our methods will help to shed exacting light on the structural changes in the pure-point spectrum at the onset of chaos.
(4) Development of a self-contained software package with a Matlab front-end, that will construct the pure-point spectrum of a given arbitrary order parabolic operator. This package will be published and freely available to end-users and beneficiaries.

From a broader perspective, the work in this proposal is intimately linked to the emerging field of geometric integration, which plays an important role in a broad array of disciplines, most notably in Hamiltonian mechanics, quantum field theory and nuclear magnetic resonance (NMR) spectroscopy. As a result of this project, new integration techniques will be realized which will directly influence the work of the beneficiaries of this research through more accurate and efficiently available information. We hope that they will not only benefit from our research and insights into achieving efficiency for such calculations, but on a more practical and direct level, that they will regularly use the software package we develop.

Host institution. The Department of Mathematics at Heriot-Watt University was rated 5 for Applied Mathematics in the last Research Assessment Exercise and has a strong emphasis in areas of direct relevance to this project: differential equations, mathematical biology, mathematical physics and numerical analysis. Professors Brown, Carr, Eilbeck, Johnston, Lacey and Sherratt in the Mathematics Department are internationally leading experts in these topics. The department has an excellent record managing research projects. Currently there are four advanced fellows, several EPSRC supported postdoctoral research assistants, and a

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number of EU research fellows. Many members of the of the department are, or have recently been involved with, seven international research networks, including the EU Reaction-Diffusion Network. The Mathematics Department is home to the Centre for Mathematical Modelling in Medicine and is a founder member of the International Centre for Mathematical Sciences (ICMS) which regularly hosts international workshops. The department also participates in the activities of the Edinburgh Mathematical Society and the Royal Society of Edinburgh and is a member of the European Consortium for Mathematics in Industry (ECMI)—two recent Teaching Company Schemes won prizes for the Best Application of Technology and Knowledge. Lastly, the department has a well managed network of Unix workstations and a substantial library with subscriptions to the journals relevant to this project.

Workplan. The individual tasks composing this project can be roughly sectioned into six month and one year long intervals, as shown in the diagram. It is expected that in the first six months to first year, the principal investigator will have a much more hands-on involvement in the project, bringing the postdoctoral researcher up-to-speed on the project background and familiarising them with some software already developed by the principal investigator and Marcel Oliver in Mathematica. After the first year the postdoctoral researcher will be expected to assume some measure of autonomy, however, towards the end of the project in the final year, the principal investigator will again become more involved to ensure the quality and completion of the project.

Activity	Personnel	6	12	18	24	30	36
$\mathcal{A}$	RA	****					
Task #1	PI & RA	****	****				
Task #2	PI & RA		****	****			
Task #3(a)	RA			****			
Task #3(b)	RA				****		
Task #4	PI & RA				****	****	
Task #5	PI & RA					****	
$\mathcal{B}$	PI & RA			****	****	****	
$\mathcal{C}$	RA		*	*		*	
$\mathcal{D}$	PI						****

Table 1. Diagrammatic workplan: with time-scale in months across the top.

Key:
$\mathcal{A}$ = Familiarisation period, knowledge transfer and literature review;
$\mathcal{B}$ = Preparation of publications and conference presentations;
$\mathcal{C}$ = Week-long visits by the RA to Marcel Oliver at the International University Bremen;
$\mathcal{D}$ = Completion of outstanding tasks and project evaluation.

Milestones.

6 Months. RA up-to-speed on geometric integration and Evans function calculations.

12 Months. Full error analysis complete. Flop count comparison and scalability assessed.

18 Months. Application to benchmark study of pulse-splitting instability and comparison in this context complete. Write-up of full error and scalabilty analysis.

24 Months. Spectral study of chaotic pulses finished. Write-up of spectral analysis application.

30 Months. Software package complete, user-ready and submitted for publication. Further analytical implications assessed.

36 Months. Complete research publications on all tasks.

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