# Description of the project:
# Group actions in function approximation spaces

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This project concerns applications of continuous (Lie) group actions on function approximation spaces. The single most important application envisaged in the course of the grant is to variational problems which have an inbuilt symmetry – specifically, to embed conservation laws exactly into numerical code.

Variational problems are endemic throughout physics and engineering.

> "Principles of optimisation such as minimum time, minimum flow resistance and minimum power expenditure have been invoked through the history of science and common speech . . . The deterministic success of these principles has become so routine that success is taken for granted." A. Bejan, *Shape and Structure, from Engineering to Nature*, Cambridge University Press, Cambridge, 2000.

Variational problems with a continuous symmetry group have guaranteed conservation laws. The PI has been concerned about automatically embedding conservation laws into numerical code ever since speaking to a Met Office mathematician, (Ian Roulstone, now at Surrey). She was told that the reason the Met Office failed to predict the 1987 hurricane was decided, after due investigation, to be that the relevant numerical models did not preserve potential vorticity.

*The 1987 Hurricane: code that incorporated potential vorticity could have predicted it*

Potential vorticity is a conservation law arising via Noether's Theorem from the particle relabelling symmetry; a rather subtle and seemingly non physical pseudogroup action. It is not at all obvious how to incorporate into a numerical model, in a bona fide way, such a conservation law. If one stops to think about it, it is not obvious how to incorporate even a simple conservation law like angular momentum. Even now, how to solve numerically the rigid body equations is still a subject of active research (even though Euler found the equations in the 1700's!) albeit as a prototype problem. While incorporating potential vorticity exactly into numerical code is a "holy grail", along the way there should be a wide range of applications whose impact is assured although the specifics can only be conjectured at present.

As computers become faster, it becomes feasible to use code that in earlier times would have been deemed too expensive in time and memory required. This is the premise of the growing field of geometric integration, which offers significantly improved qualitative information (at a minimum) in the numerical integration of differential systems.

# 1 Mathematical Background

The project builds on classical Calculus of Variations and modern function approximation methods. The main novel techniques used are moving frames and discrete variational methods. The overall context is geometric integration, an increasingly hot topic in numerical analysis.

## Moving Frames

Sophus Lie famously introduced and applied smooth group actions to differential systems from the early 1870s to the late 1890s. Tresse used the invariants of such actions to study the equivalence problem for ordinary differential equations in a prize-winning essay in 1896. This extraordinary work has assumed new importance in the search for on-line symbolic integrators of nonlinear ordinary differential equations, such as Maple's `dsolve`. Cartan famously applied the notion of a moving frame to solve higher dimensional equivalence problems in differential geometry, relativity, and so on (1920s and 1930s). Moving frames were further developed and applied in a substantial body of work, within differential geometry and using mostly exterior differential calculus as the preferred language, see for example papers by Bryant, Green and Griffiths (1970s and 1980s).

A breakthrough in the understanding of moving frames came in a series of papers by Fels and Olver in 1998 and 1999, which provide a coherent, rigorous and constructive moving frame method free from any particular set up, and hence applicable to a huge range of examples, from classical invariant theory to numerical schemes. There have already been applications to discrete spaces; to computer vision (for example, [4]) and to invariant numerical schemes [11].

To date the main application of moving frames to function approximation is the multi-space construction [17] with which the PI has some experience [14].

## Discrete Variational Methods ...

Variational principles are a central concept in the analysis of physically important models, and for systems described by differential expressions, the Calculus of Variations is a mature subject. The systematic study of Lagrangians and the derivation of Euler-Lagrange operators for *difference systems* is relatively recent, dating from the 1980's (Maeda and Kuperschmidt).

A variational calculus is formulated in terms of an "exact differential complex"; the most famous example of this concept is the grad-curl-div sequence of operators. Exactness means that if one operator in the sequence sends an expression to zero, then that expression is in the image of the previous operator in the sequence. Thus, if the curl of a vector field is zero, then locally it is the gradient of a function. The extended sequence grad-curl-div-Euler Lagrange-Helmholtz is still exact, and is known as the continuous variational complex.

It is now recognised that for a stable numerical scheme, it is important to mimic this exactness.

> "In many contexts it is not enough that the numerical scheme be close to the original problem in a quantitative sense for it to inherit stability ... the exactness properties of discrete differential complexes and their relation to differential complexes associated with the PDE are crucial tools in establishing the stability of numerical methods." [1]

## ... and function approximation

The complexes used by Arnold, Falk and Winthur [2] involve polynomial function spaces of various kinds. These are related to constructions of so-called "Whitney forms" [3] which at low order are in fact simplicial approximations coming from classical algebraic topology. There is a lot of research activity in the general area of "discrete differential forms", for example by Marsden and his co-workers, and more under the titles "mimetic methods", "finite volume" and others, with problems in the numerical solution of Maxwell's equations being a big motivating factor.

Also of interest are splines, wavelets and frames [6]. A student of the PI, Jun Zhao, has developed a discrete variational calculus for spline based approximations.

## ... and Noether's Theorem: The Challenges

One of the most important applications of having a precisely formulated variational structure is Noether's Theorem. This result allows one to deduce conservation laws from symmetries, illustrated schematically in Figure 1. The application of Noether's Theorem consists in the smooth classical case of a recipe for manipulating differential equations. The challenge is thus, what should replace this when we have only columns of numbers?

**Symmetry** ⟶ **Noether's Theorem** ⟶ **Conservation Law**

Figure 1: Challenge One: What replaces the black box for numerical data?

Some examples studied in physics and engineering are

| **Symmetry** | **Conservation Law** |
|---|---|
| Translation in time | Energy |
| Translation in space | Linear momentum |
| Rotation in space | Angular momentum |
| Particle relabelling | Potential vorticity |

The list shows that the symmetries often involve actions in the base space; but the base space is what is discretised! This intellectual challenge is illustrated in Figure 2.

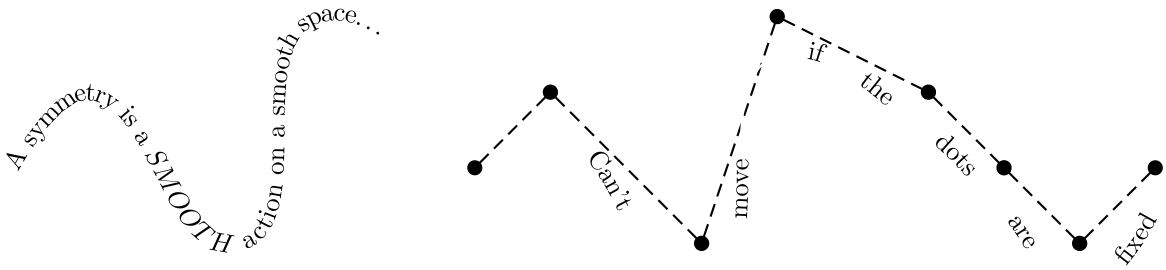


Figure 2: Challenge Two: what replaces group actions on the base space after it is discretised?

**Solutions to the challenges** *The solution to the Challenges* is to induce the group action on the moments used in the function approximations. This works because you can replace expressions in standard differential terms by expressions in moments in the formulae that Noether's Theorem gives you. Specifically: the PI's idea in (Track record, [3]) was to replace the "web" of concepts and their relationships that underpin the proof of Noether's Theorem, with an analogue suitable for the function approximation space at hand. This is illustrated schematically in Figure 3. The top diagram is the part of the variational complex used to derive Noether's Theorem for smooth differential Lagrangians [15]. The second is the analogue for Finite Element developed by the PI in discussion with Reinout Quispel. The analogue builds on work by Douglas Arnold (Minnesota) and co-workers, who show that the relevant concepts in the left half of the web have meaning for users of Finite Element approximations. Approximations that fit the left half are guaranteed to be numerically stable [1]. The right half gives the structure needed for the variational calculations. The proof of Noether's Theorem requires the join of the two halves.

SMOOTH

$$\begin{array}{ccccccccc} \stackrel{\mathrm{Curl}}{\rightarrow} & \Lambda^2 & \stackrel{\mathrm{Div}}{\rightarrow} & \Lambda^3 & \stackrel{\hat{\mathrm{d}}}{\rightarrow} & \hat{\Lambda}_1 & \stackrel{\hat{\mathrm{d}}}{\rightarrow} & \hat{\Lambda}_2 & \stackrel{\hat{\mathrm{d}}}{\rightarrow} \\ & & & & & \downarrow \pi & & \downarrow \pi & \\ & & & & & {\Lambda^1}_* & \stackrel{\delta}{\rightarrow} & {\Lambda^2}_* & \stackrel{\delta}{\rightarrow} \end{array}$$

Finite Element

$$\begin{array}{ccccccccc} \stackrel{\mathrm{d}}{\rightarrow} & \widetilde{\mathcal{F}}^2 & \stackrel{\mathrm{d}}{\rightarrow} & \widetilde{\mathcal{F}}^3 & \stackrel{\hat{\mathrm{d}}\circ\int}{\rightarrow} & \widehat{\mathcal{F}_1} & \stackrel{\hat{\mathrm{d}}}{\rightarrow} & \widehat{\mathcal{F}_2} & \stackrel{\hat{\mathrm{d}}}{\rightarrow} \\ & & & & & \downarrow \pi & & \downarrow \pi & \\ & & & & & \mathcal{F}^1_* & \stackrel{\delta}{\rightarrow} & \mathcal{F}^2_* & \stackrel{\delta}{\rightarrow} \end{array}$$

Figure 3: Conceptual pattern matching to create a variational complex

*All in all, the interpretation and implementation of the extremely theoretical result in (Track record, [3]) for particular function spaces and their numerical representation, is needed. This is the part that needs work: from intuiting how to solve a problem to actually carrying it out in a practical way is a large step requiring new ideas, time and resources.*

**Geometric Integration** is concerned with the idea that discretisations should inherit the *structure* of the original model; the idea is philosophically attractive and increasingly popular. "Structure" includes concepts like symmetry, a symplectic form, or first integrals [13]. There are two approaches to the numerical solution method for variational problems with a Lie group symmetry:

- The first is to study a related discrete variational problem, one that has both the correct continuum limit and the group invariance built in from the start. By virtue of a discrete Noether's theorem, this ensures the existence of a matching discrete conservation law with no further effort on the part of the programmer. A recent paper where this principle is applied (by bona fide numerical analysts and physicists) is [7].
- The second is to consider the general class of invariant differential systems, which include Euler Lagrange equations arising from an invariant Lagrangian. Such systems can be analysed using moving frames which provide a "divide and conquer" solution mechanism. The pieces are (i) the evolution of the invariants, and (ii) an evolution in the group of the form,

$$\rho_s = A\rho \tag{1}$$

where $A$ is in the relevant Lie algebra whose components are invariants, and $s$ is an independent variable. Some applications, especially in integrable systems, are concerned only with the evolution of the invariants, while others, such as mechanics (e.g. spinning tops) are concerned solely with the evolution in the group. But in general, both evolutions are important. The classical Lie group reduction techniques work for one-dimensional continuous group actions and more generally, *solvable* Lie groups, while the PI has shown that moving frames work, in principle, for arbitrary Lie symmetry groups (Track record, [1]).

The numerical integration of equations of the type (1) have been intensively studied [10]. However, the results thus far are for the *initial value problem*, while variational problems tend to be boundary value problems.

## 2 Long term Aims of the line of research of this Project

This project is the first step to achieving these long term aims:

Aim 1 Commercial numerical code that incorporates conservation laws of variational systems *exactly*, by virtue of incorporating the symmetries that give rise to the conservation laws, into the corresponding discretised variational model. *Please see the Impact Plan.*

Aim 2 Commercial numerical code that incorporates the foliated nature of the solution set of a Lie group invariant differential equation *exactly*, by virtue of incorporating the symmetries that give rise to the foliation, into the discretisation.

First must come the mathematics, then "in principle" code with worthwhile examples, then efficient code. Specifically, what is needed first are coherent, accessible, practical and philosophically well grounded accounts to be developed and written of

1. the mathematics of Lie group actions on function approximation spaces, for example, those used in Arnold et al's discussion of the Finite Element method [2],

2. the theorems yielding discrete versions of Noether's Theorem, in particular how they may be understood in the computational sense

3. the solution of equations of the type (1) when the components of $A$ are known only in terms of a given function approximation space.

# 3 Programme and Methodology

The proposal mostly is about achieving short term objectives that will help achieve Aim 1 above. The logical order of events is as follows:

Obj. 1 Develop and write a coherent, practical account of Lie group actions on function approximation spaces. Investigate examples of invariants and relations the invariants satisfy, and how these invariants are used. This is necessary because the PI couldn't find one.

Obj. 2 Develop and write a coherent and practical account of the application of moving frames to obtain new theorems about invariants of Lie group actions on function approximation spaces.

Obj. 3 Develop and then write a coherent and practical account of the analogue of Noether's Theorem for finite element discretisations of variational problems.

Obj. 4 Investigate in detail worthwhile examples, complete with coding and computer generated results and graphics.

Obj. 5 Write and make publically available, code that works on a variety of inputs that uses the new ideas developed during the course of the project.

While there is a *theoretical* account of Noether's Theorem for finite element discretisations of variational problems, (Track record, [3]), it is far from being practical. A whole second set of ideas is needed.

The PI and PDRA will collaborate on solving the mathematical problems inherent in Objectives 1-3. The PDRA will then work on Objectives 4 and 5 while the PI concentrates on communicating the mathematical results to an audience broader than that of the immediate research papers. Finally, the calculations on practical examples will be communicated.

## 3.1 Relevance to Academic Beneficiaries

The academic beneficiaries will be researchers in a wide range of engineering and mathematical fields.

Increasingly, researchers are looking for ways of how to include into a discretisation, a wide variety of geometric structures enjoyed by the continuous mathematical models. Symmetries abound in nature, such as translation in time and space, rotation in space, pseudo-rotations in space-time, with scaling symmetries, particle relabelling symmetries and so forth also common. Usually, these symmetries are built into the continuous mathematical models but not their discretisations, because no-one knows how to do it, at least, not algorithmically.

Symmetries of finite difference variational problems have been well investigated in the last decade, the most general results to date being in [9], but have been mainly taken up by people interested in integrable systems.

The idea to build symmetry into more sophisticated numerical schemes for variational problems is starting to be taken up by numerical analysts and physicists, see for example [7]. This project proposes to develop a largely algorithmic approach to incorporating into discretisation schemes currently in use, those conservation laws arising from symmetries for variational problems. This includes a wide variety of conservation laws for physical problems.

While rooted in classical applied analysis, the project builds on work which has appeared only in the last 10 years. The seminal papers by Fels and Olver [8] on the moving frame method appeared in 1998-99, while the Kogan and Olver paper [12] on the invariantized variational complex appeared in 2004. The PI's paper on Noether's theorem for finite difference and finite element Lagrangians appeared in 2006 (Track record, [4]), while her simplified derivation of invariant Euler Lagrange equations is to appear (Track record, [1]).

## Relevant Bibliography from the PI's Track Record


1. E.L. Mansfield, A practical guide to the invariant calculus, Cambridge University Press, in press. `http://www.kent.ac.uk/ims/personal/elm2/FrameBook2Jun09.pdf`
2. — and P.E. Hydon A variational complex for difference equations *Foundations of Computational Mathematics* (2004) 4187–217
3. — and G.R.W. Quispel, Towards a variational complex for the Finite Element Method *Group Theory and Numerical Analysis* (2005) CRM Lecture Notes and Proceedings **39** 207–231
4. —, *Noether's Theorem for Smooth, Difference and Finite Element Systems*, in Foundations of Computational Mathematics, Santander, 2005, Editors: Pardo, Pinkus, Süli and Todd, CUP 2006.
5. — and P.E. Hydon, *Difference Forms*, *Foundations of Computational Mathematics* (2008) 8427–467
6. —, Algorithms for symmetric differential systems *Foundations of Computational Mathematics*, 1, 2001, 335–383
7. —, N. Bila and P.A. Clarkson, Symmetry Group Analysis of the Shallow Water and Semi-Geostrophic Systems *Quarterly Journal of Mechanics and Applied Mathematics*, (2005)
8. — and P. van der Kamp, Evolution of curvature invariants and lifting integrability *J. Geometry and Physics* (2005) 56 1294–1325
9. E. Shemyakova and —, Moving frames for Laplace Invariants, in ISSAC '08 (an international refereed conference).


## References


[1] D. Arnold, (2002), *Differential complexes and numerical stability*, Proceedings of the International Congress of Mathematicians, Beijing 2002, Volume I: Plenary Lectures. `http://www.ima.umn.edu/~arnold/papers/icm2002.pdf`

[2] D. Arnold, R.S. Falk and R. Winther (2006), Finite element exterior calculus, homological techniques, and applications, Acta Numerica, **15** 1–155.

[3] A. Bossavit (2002), Generating Whitney forms of polynomial degree one and higher, IEEE Trans. Magnetics, **38**(2) 341–344.

[4] M. Boutin (2003), Polygon recognition and symmetry detection, *Found. of Comp. Math* **3** 227–271

[5] P.A. Clarkson and P.J. Olver (1996), Symmetry and the Chazy equation *J. Diff. Eq.* **124** 225–246.

[6] Ole Christensen, *An Introduction to Frames and Riesz Bases (Applied and Numerical Harmonic Analysis)*, Birkhauser, 2002.

[7] S. Christiansen and T.G. Halvorsen, Solving the Maxwell-Klein-Gordon equation in the Lattice Gauge Theory formalism, IMA J. Numer. Anal. to appear.

[8] M. Fels and P.J. Olver, Moving Coframes I and II, (1998-9) *Acta Appl. Math.* **51** 161–213; **55** 127–208.

[9] M. Hickman and W. Hereman (2003), Computation of Densities and Fluxes of Nonlinear Differential-Difference Equations, Proceedings Royal Society of London A, **459**, pp. 2705–2729.

[10] A. Iserles, H.Z. Munthe-Kaas, S.P. Nørsett, A. Zanna (2000), Lie group methods, Acta Numerica **9** 215–365.

[11] P. Kim, Invariantization of Numerical Schemes Using Moving Frames, (2007), BIT Numerical Mathematics 47(3) 525–546.

[12] I.A. Kogan and P.J. Olver (2003), Invariant Euler-Lagrange equations and the invariant variational bicomplex *Acta Appl. Math.* **76** 137–193.

[13] R.I. McLachlan, G.R.W. Quispel, Six lectures on the geometric integration of ODE's, in: R.A. DeVore et al. (Eds.), Proceedings of the International Conference on Foundations of Computational Mathematics, C.U.P., 2001.

[14] E.L. Mansfield and P.E. Hydon, Towards approximations which preserve integrals ISSAC (2001), Editor B. Mourrain, ACM Publishing 217–222

[15] P.J. Olver, *Applications of Lie Groups to Differential Equations*, Springer Verlag, Second Edition, 1993.

[16] P.J. Olver (2001) Joint invariant signatures *Found. of Comp. Math* **1** 3–67.

[17] P.J. Olver (2001), Geometric foundations of numerical algorithms and symmetry *App. Alg. Eng. Comm. Comp.* **11** 417–436