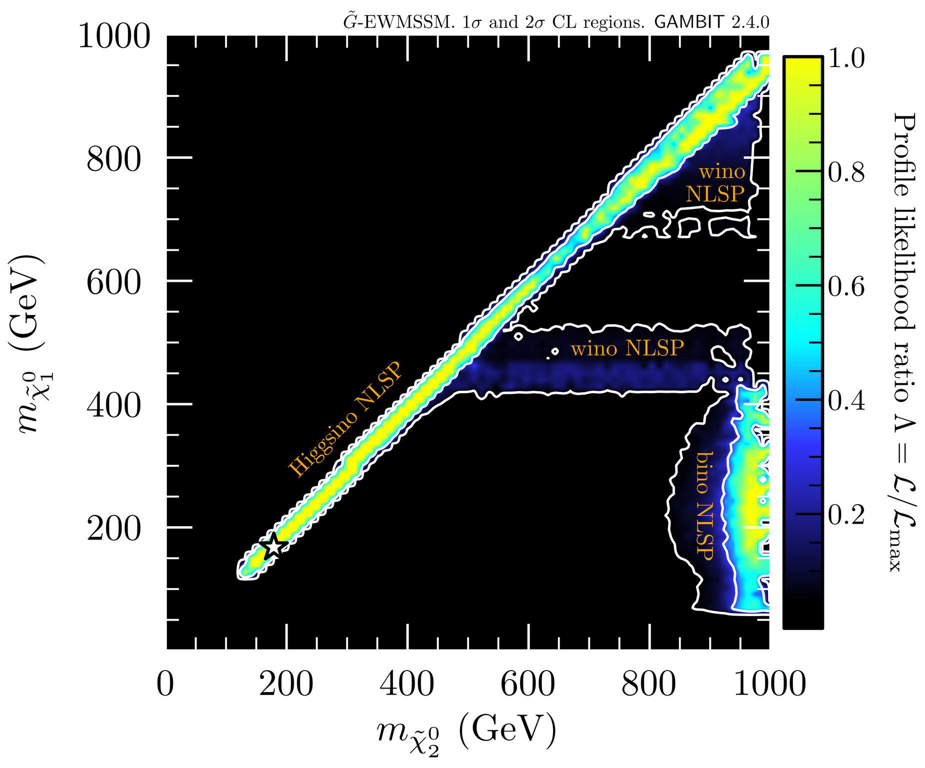
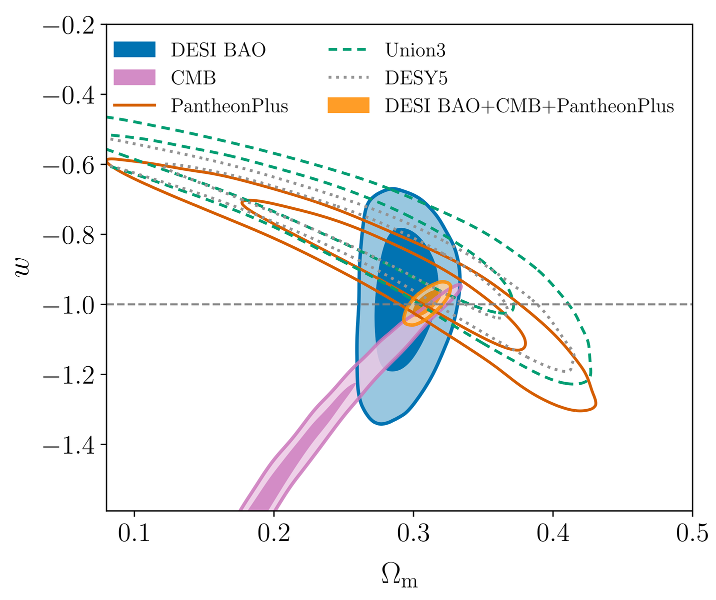
INFERENCE

Fundamental physics is full of hard inference problems. Our optimization or sampling algorithms have to be able to navigate complex geometry



Gambit Collaboration SUSY profile likelihood scan[1]

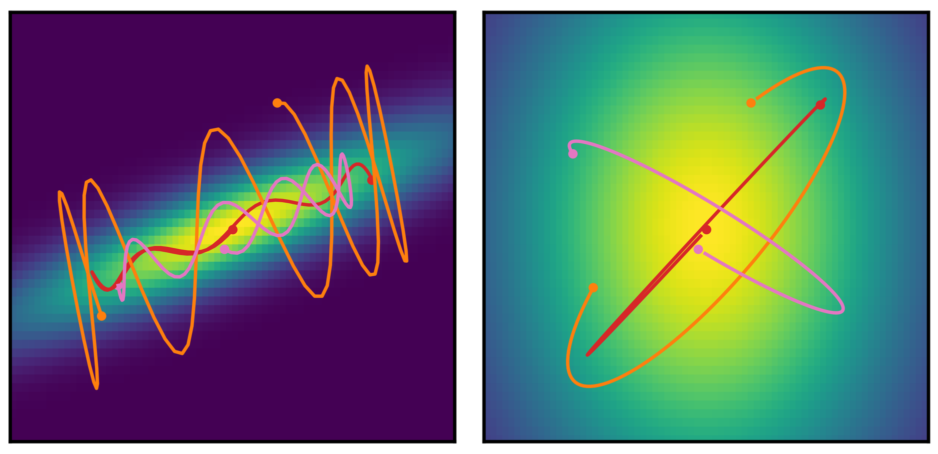


DESI collaboration LCDM samples[2]

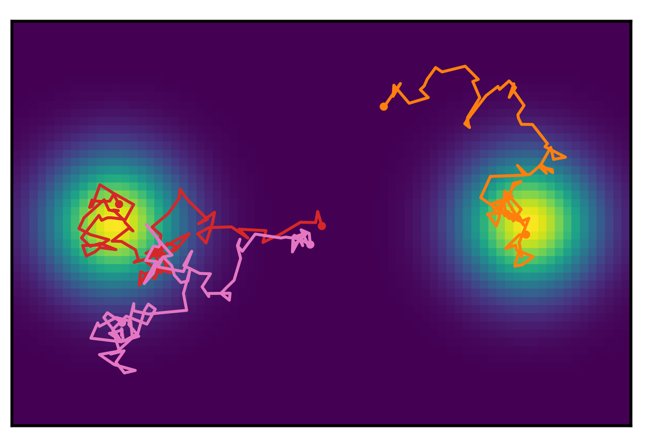
GEOMETRY

Bad geometry[3] in inference problems comes in many guises, and intuition gets progressively less clear in high dimension. Machine learnt neural mappings offer us a new tool to approach this.

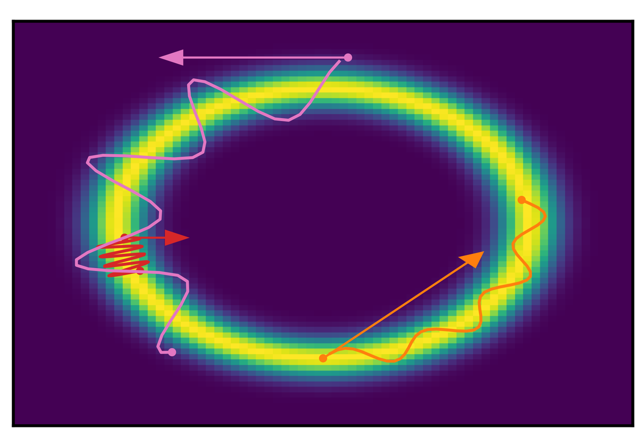
In the context of bridging distributions see `pocoMC`[4], `nessai`[5]



Whitening transforms to regularize the metric.



Clustering/ensembling to deal with multimodalities.



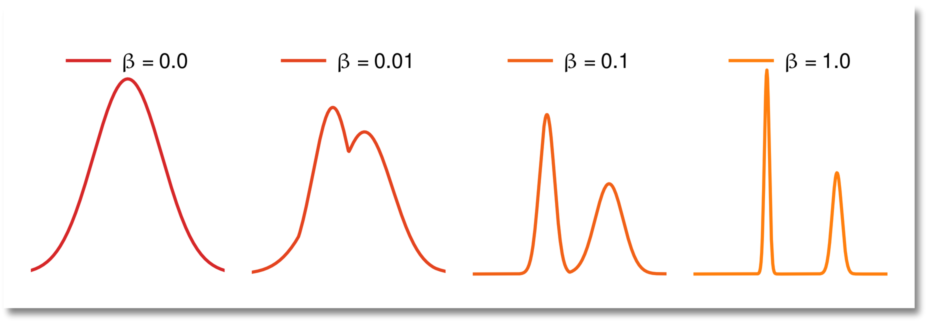
Gradients efficiently explore sweeping degeneracies.

BRIDGING DISTRIBUTIONS

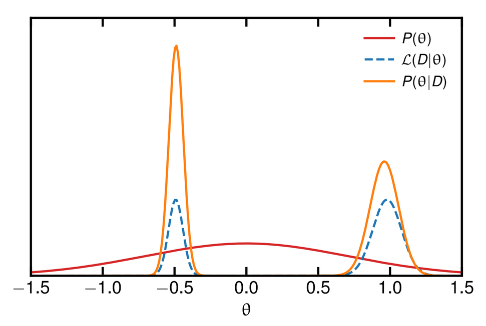
Population Monte Carlo methods — particle filters — form bridges from known (prior) to complex unknown (posterior) distributions. Sequential Monte Carlo (SMC) and Nested Sampling (NS) are two variants evolving populations of points[6]. Both give us access to the normalizing constant Z.

$$P(\theta\,|\,D) = \frac{\mathscr{L}(D\,|\,\theta)P(\theta)}{Z}$$

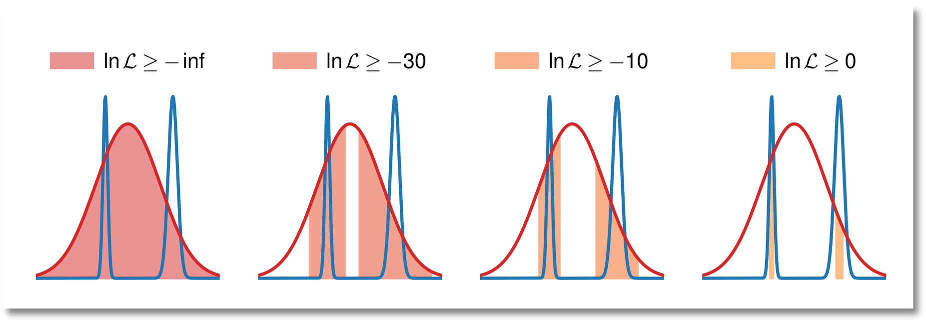
Bayes Rule



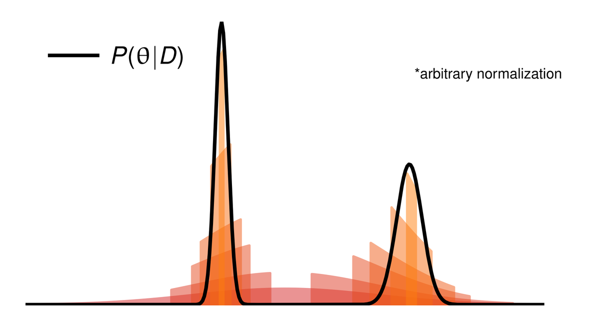
SMC



Toy 1D inference problem.



NS

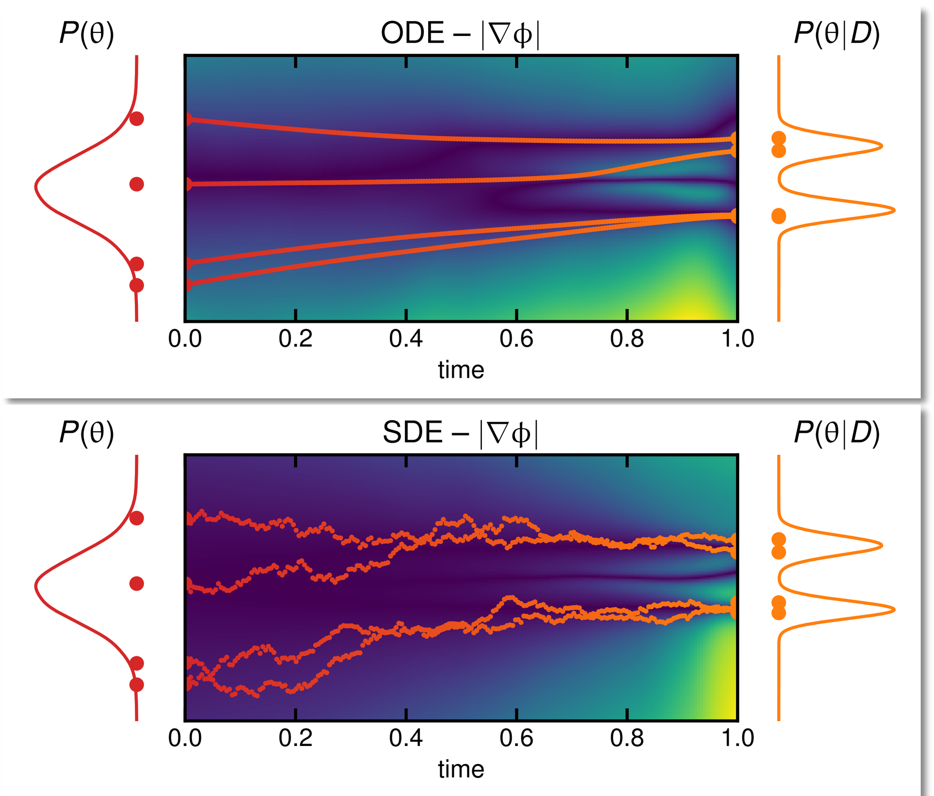


Schematic reconstructing posterior from NS shells.

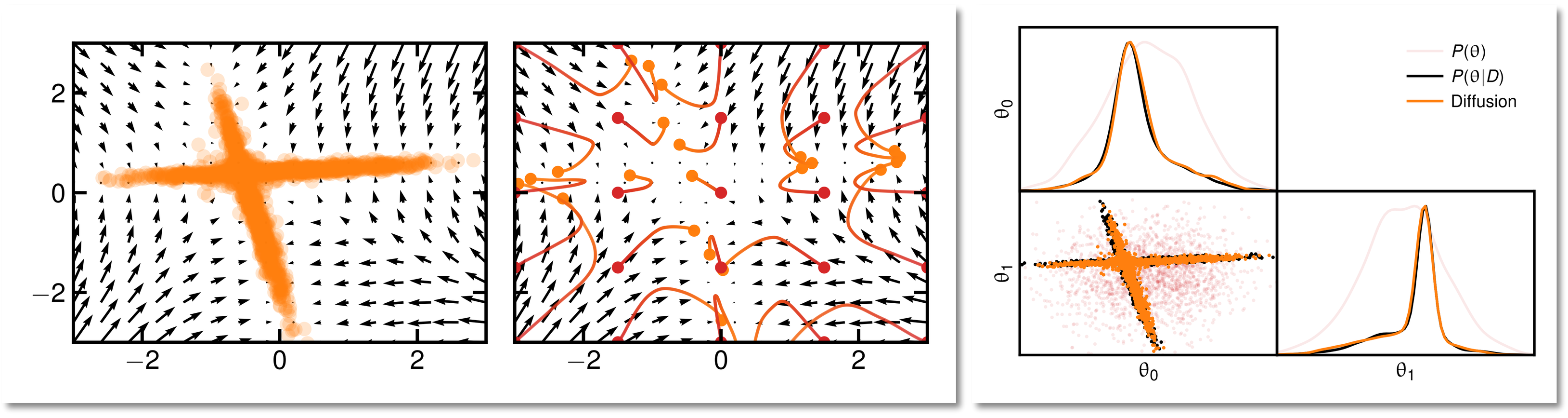
DIFFUSION

Diffusion models learn the gradient of the implicit density of a point cloud. Solving evolution through this field with Stochastic Differential Equation (SDE) or Ordinary Differential Equation (ODE) solvers yields Diffusion[7] or Continuous flows[8].

Neural learnt maps can transport any known distribution to an implicit target, no strict requirement on latent/prior!



Learnt gradient vector field mapping prior to posterior.



2D representation of learnt vector fields.

DIFFUSION MEETS NESTED SAMPLING

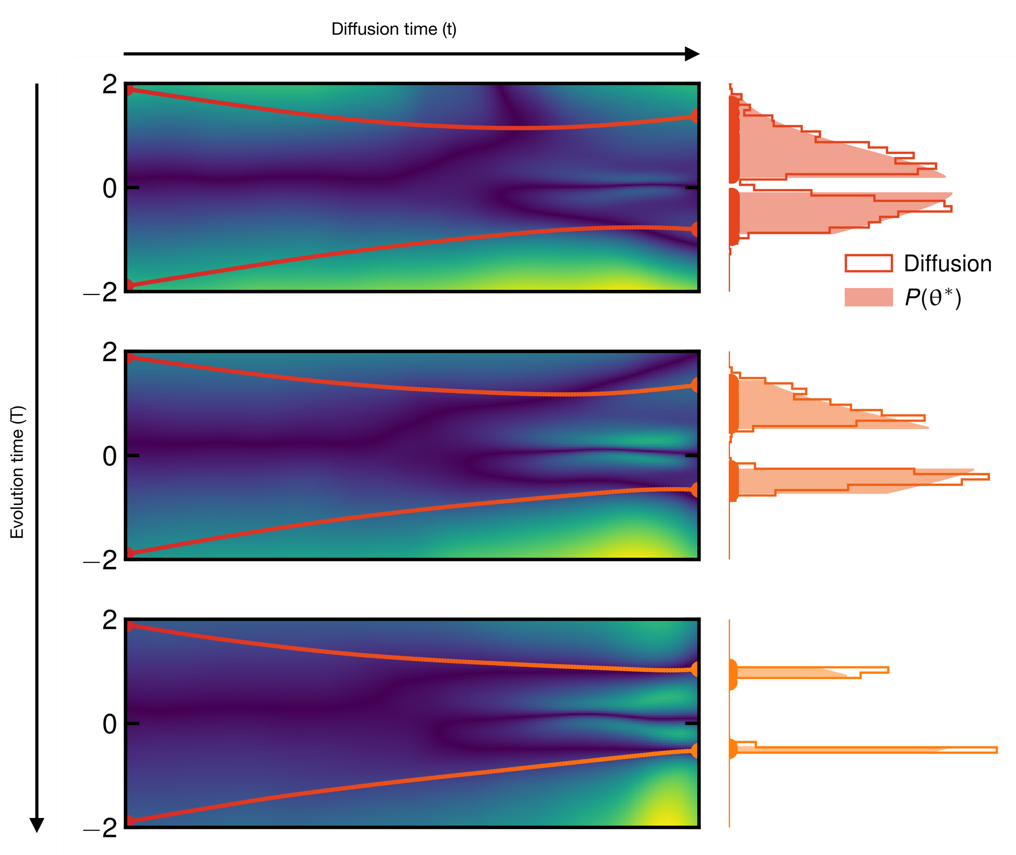
NEUTRALISING BAD GEOMETRY IN BRIDGING INFERENCE PROBLEMS

DAVID YALLUP

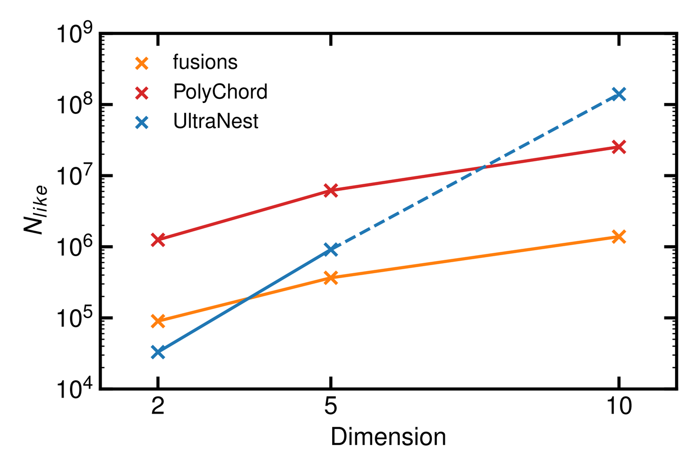
yallup/fusions dy297@cam.ac.uk yallup@github.io

RESULTS*

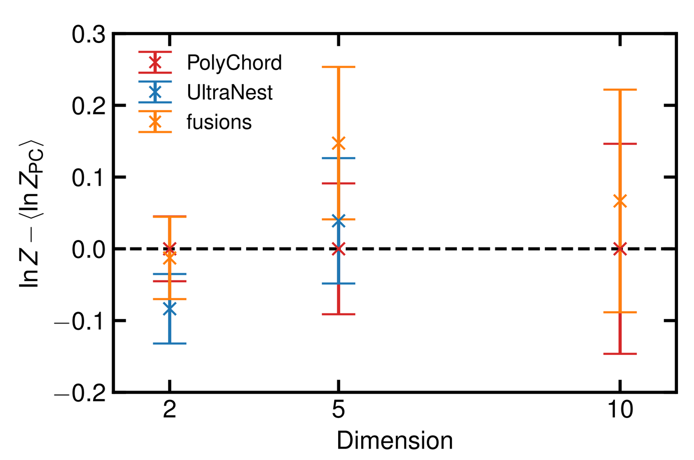
Diffusion models introduce time axis to the problem, bridging algorithms have another time axis we can efficiently evolve by fine tuning the score estimate.



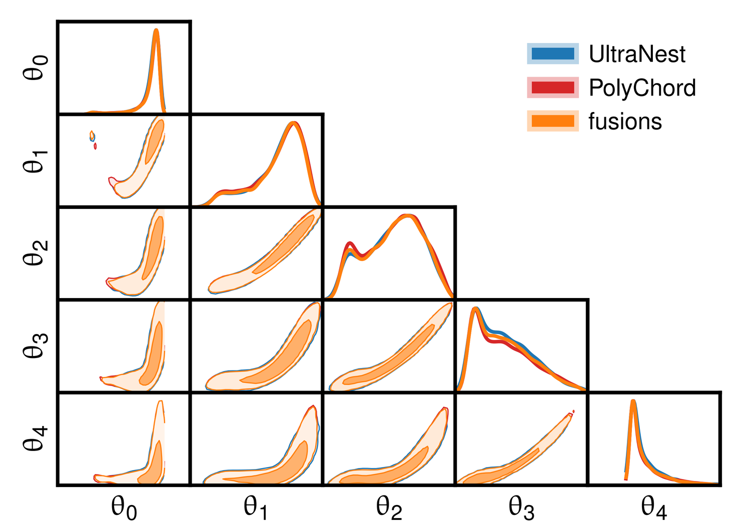
Evolution of likelihood constrained prior through a NS run.



Number of function evaluations required for Rosenbrock function in various dimensions



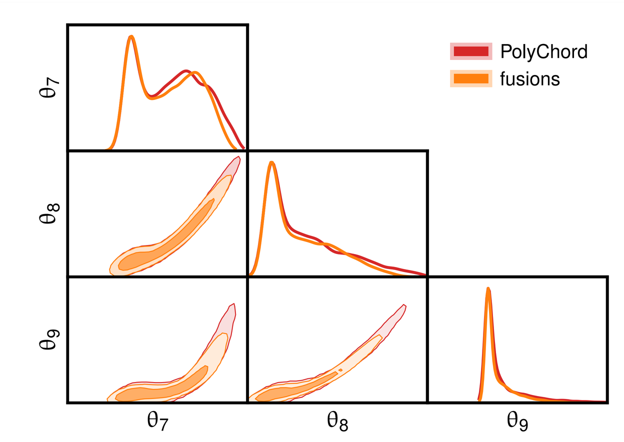
Calculated log integral for Rosenbrock function in various dimensions



Corner plot of 5D Rosenbrock function

$N_{\rm live} = 2000$ for all, otherwise following defaults.

UltraNest in 10D $N_{\rm like}$ projected after early termination due to exceeding walltime.



Partial corner plot of 10D Rosenbrock function

Comparison to standard (non-neural) tools[9,10] shows promising scaling, comparable to step samplers despite using rejection sampling, whilst maintaining accurate predictions on benchmark challenging problems.

Algorithm demonstrated uses *zero* classical methods, treating the geometry of the problem solely with neural networks and score based models.

* Work in progress, comparison to other neural methods[4,5,11,12], plenty left on the table to tune in the algorithm.

References:

1.[2303.09082] The Gambit collaboration
2.[2404.03002] DESI Collaboration
3.[1903.03704] Hoffman et al.
4.[2207.05660] Karamanis et al.
5.[2102.11056] Williams et al.
6.[2205.15570] Ashton et al.
7.[2011.13456] Song et al.
8.[2302.00482] Tong et al.
9.[2101.09604] Buchner
10.[1506.00171] Handley et al.
11.[2306.16923] Lange
12.[1903.10860] Moss

Technical references:
- github.com/patrick-kidger/diffrax
- github.com/handley-lab/anesthetic
- github.com/yallup/fusions
- github.com/google/flax
- github.com/google/jax

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