

Essential Tools for Scientific Machine Learning and Scientific AI | Comparison of tools readily usable with differentiable programming (automatic differentiation) frameworks

Subject AD Frameworks	ADIFOR or TAF	ADOL-C	Stan	Julia (Zygote.jl, Tracker.jl, ForwardDiff.jl, etc.)	TensorFlow	PyTorch	Misc. other good packages
Language	Fortran	C++	Misc.	Julia	Python, Swift, Julia, etc.	Python	
Neural Networks	neural-fortran	OpenNN	None	Flux.jl	Built-in	Built-in	ADIFOR
Neural Differential Equations	Sundials (ODE+DAE)	Sundials (ODE+DAE)	Sundials (ODE+DAE)	DifferentialEquations.jl / DiffEqFlux.jl (ODE, SDE, DDE, DAE, hybrid, (S)PDE)	DifferentialEquations.jl (through Tensorflow.jl)	torchdiffeq (non-stiff ODEs)	PyMC3 (Python)
	FATODE	PETSc TS	Built-in (non-stiff ODE)	Sundials.jl (ODE through DiffEqFlux.jl)		diffeqpy	SMT (Python)
Probabilistic Programming	None	CPPProb	Built-in	Gen.jl	Edward	Pyro	sensitivity (R)
				Turing.jl	PyMC4	pyprob	ColPACK (Fortran)
Sparsity Detection	Built-in (TAF)	Built-in	None	SparsityDetection.jl	None	None	Dakota
Sparse Differentiation	Built-in (TAF)	Built-in	None	SparseDiffTools.jl	None	None	PSUDAE
GPU Support	CUDA	CUDA	OpenCL	CUDANative.jl + CuArrays.jl	Built-in	Built-in	Mondrian
Distributed Dense Linear Algebra	ScaLAPACK	Elemental	None	Elemental.jl	Built-in	torch.distributed (no factorizations)	SimLab (MATLAB)
				DistributedArrays.jl		Elemental	Halide
Distributed Sparse Linear Algebra	ScaLAPACK	PETSc	None	Elemental.jl	Built-in (no factorizations)	Elemental	dolfin-adjoint (AD for FEniCS/Firedrake)
	PARASOL	Trilinos		PETSc.jl	None	petsc4py	
		Elemental			None		
Structured Linear Algebra	SPARSEKIT	None	None	(Block)BandedMatrices.jl	Some built-in	None	
Surrogate Modeling	None	MUQ	None	Surrogates.jl	None	pySOT	
Global Sensitivity Analysis	None	None	None	DifferentialEquations.jl / DiffEqSensitivity.jl	None	SALib	
Uncertainty Quantification	None	MUQ	None	DifferentialEquations.jl / DiffEqUncertainty.jl	None	uncertainpy	
Direct Distributed Parallelism	MPI	MPI	MPI	MPI.jl	Built-in	torch.distributed	
PDE Discretizations	C++ Libraries w/ Fortran interfaces (hypr)	deal.ii	None	ApproxFun.jl		FEniCS	
		SAMRAI		DiffEqOperators.jl		Firedrake	
		hypr		JuAFEM / JuliaFEM		Dedalus	

Note: these statements/ratings are all about AD compatibility and usability for scientific machine learning and not necessarily applicable to traditional machine learning

For more details, see <http://www.stochasticlifestyle.com/a-comparison-between-differential-equation-solver-suites-in-matlab-r-julia-python-c-and-fortran>

Scale	None	Poor	Fair	Excellent
Explanation	No automatic differentiation compatible library exists. Suggestion for a library to wrap.	Functionality exists, but is feature-incomplete or AD compatibility is incomplete. If no AD support, then AD support can easily be added since the library already defines adjoints.	The basic features exist, but has some major features missing or are not AD-compatible.	Has all of the main features and is fully compatible with the automatic differentiation tooling.