

Kokkos Kernels: ODE

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Recall the structure of ODEs

$$\frac{\partial y}{\partial t} = f(y, t), \quad y(0) = y_0$$

Two major families of solvers can be used

1. Explicit time integrators

- ▶ Only require function evaluations and vector operations
- ▶ Easy to implement, flexible order of integration
- ▶ Require small time step for appropriate convergence (CFL condition)
- ▶ Can easily support adaptive time stepping

2. Implicit time integrators

- ▶ Requires Jacobian evaluation and non-linear solver
- ▶ Can be time-step and order adaptive but needs a complex control flow
- ▶ Uses larger time-steps and can solve stiff system of equations

Primary goal is to support solution of many ODEs concurrently.

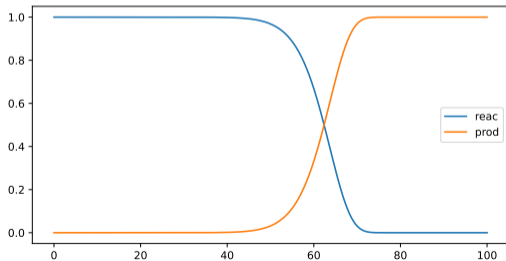
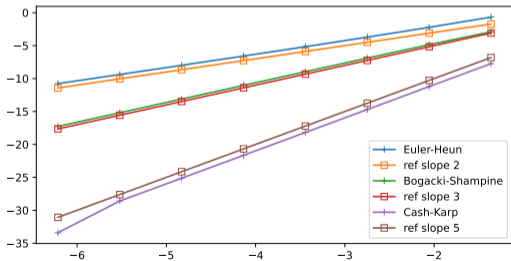
Support both explicit and implicit adaptive solvers

- ▶ Explicit Runge-Kutta order 1 to 5
- ▶ Implicit Backward Difference Formula, order 1 to 5
- ▶ Implicit Adams-Moulton orders 1 to 6 (maybe up to 12)

Single problem and batched problems interfaces

- ▶ Explicit and implicit solvers will both have single problem interface on device (callable within inner most parallel level)
- ▶ Explicit algorithms will have batched interface, implicit ones need more evaluation for batched approach

- ▶ Implementation of single problem interface complete
- ▶ All classic variants from order 1 to 5 implemented (Fehlberg, Bogacki-Shampine, Cash-Karp, Dormand-Prince)
- ▶ Batched interface and implementation underway
- ▶ Dormand-Prince 8-5-3 variant could be next feature?
- ▶ Symplectic algorithms maybe considered?



- ▶ Implementation of single problem complete
- ▶ Performance optimization still underway
 - ▶ memory foot print reduction
 - ▶ Jacobian calculation and factorization reuse
- ▶ Only dense Jacobian supported, sparse coming next

