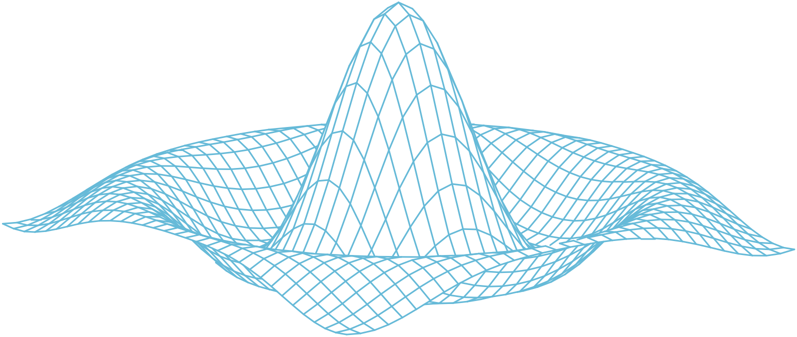
odepkg: Present and Future

TECHNISCHE UNIVERSITÄT DARMSTADT

J. Corno



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GRADUATE SCHOOL
computational engineering

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Outline

1 Release 0.8.5

2 SoCiS 2013

3 SoCiS 2014

4 TODOs and Discussion

Release 0.8.5

- Released on 19 May 2015
- Octave 4.0 compatibility (Tatsuro Matsuoka)

SoCiS 2013 (Roberto Porcù & Mattia Penati)

- **New solvers**: Geometric integrators for Hamiltonian Systems
  - **odeSE** (Symplectic Euler)
  - **odeSV** (Stormer Verlet)
  - **odeVV** (Velocity Verlet)
  - **odeSPVI** (SPectral Variational Integrator)
  - **odeRATTLE** (RATTLE algorithm)
- **New options handling**
  - **Levenshtein**
  - **Fuzzy compare**
- **New structure**
  - **Steppers**
  - **Integrate functions**

SoCiS 2013 (Roberto Porcù & Mattia Penati)

The new organization tries to subdivide the code according to the most important operations.

Optimization of the bottlenecks and **extension** of the code should be easier.

Steppers

A **stepper** executes just one integration step

```
[x_next, err] = stepper (f, x, t, dt)
```

The estimation of the error is used to determine the optimal `dt` in adaptive integrators.

Integrate Functions

Given the stepper, an **integrate function** executes the integration algorithm on more steps

- `integrate_const (stepper, f, t, x0, dt, opts)`
- `integrate_n_steps (stepper, f, t0, x0, dt, n, opts)`
- `integrate_adaptive (stepper, p, f, t, x0, opts)`

All Together: ode45

```
switch integrate_func
case 'const'
      solution = integrate_const (@runge_kutta_45_dorpri
         , fun, tvec, x0, dt, opts);
    case 'n_steps'
      solution = integrate_n_steps (
         @runge_kutta_45_dorpri, fun, t0, x0, dt, n,
         opts);
    case 'adaptive'
      solution = integrate_adaptive (
         @runge_kutta_45_dorpri, order, fun, tvec, x0,
         opts);
  endswitch
```

SoCiS 2014

- New structure for all the explicit solvers
- **odeset** and **odeget** Matlab compatible
- Implementation of the missing options (MaxStep, NormControl, etc...)
- Tests added and bugfixes
- **F**irst **S**ame **A**s **L**ast (when possible)
- Dense output

Dense Output

Provide the solution at a given time $s \in [t, t + dt]$ with the **same order of accuracy** as the solutions computed at the internal time points by using suitable interpolation methods.

- `x_out = linear_interpolation (t, x, t_out)`
- `x_out = quadratic_interpolation (t, x, der, t_out)`
- `x_out = hermite_cubic_interpolation (t, x, der, t_out)`
- `x_out = hermite_quartic_interpolation (t, x, der, t_out)`
- `x_out = dorpri_interpolation (t, x, k, t_out)`
- `x_out = hermite_quintic_interpolation (t, x, der, t_out)`

Dense Output

- 1st order approximation with no function evaluation
- 2nd order approximation may require the evaluation of the function at the current time. Avoided if the stepper already returns that value
- The only 3rd explicit order solver implemented is **ode23**. The 3rd order approximation exploits the Runge-Kutta k values to avoid further function evaluations.
- If **ode45** is used without local extrapolation then **dorpri_interpolation** gives 4th order approximation without any additional function evaluation

Dense Output

- For **ode45** with local extrapolation, Shampine proposes 4th order approximation at the middle point and to use quartic interpolation. The quintic interpolation requires an additional function evaluation without (according to Shampine) a significant improvement
- For the higher order solvers (**ode78**), a suitable interpolator has not yet been implemented

Further optimization can be performed:

- If more than one solution is requested in $s \in [t, t + dt]$
- For specific solvers

TODOs and Discussion

- Clean-up and release with the new structure (0.9.0 ?)
- Move to core the most used solvers
  - **ode45**
  - **ode23**
  - **ode23s**
  - **ode15s** (to be implemented!)
  - **bvp4c** (and other BVP?)
  - **odeset** & **odeget**

N.B. To move the main solvers to core it is necessary to move also

- The utilities for the options (**levenshtein**, ...)
- The three **integrate functions**
- The **steppers** corresponding to the solvers
- ...

TODOs and Discussion

Questions for discussion:

- **inputParser** for **odeset**/**odeget**
- When to move? Before or after new release?
- What happens to **daspk**, **dassl**, ...
  - Remove
  - Keep and change interface according to **odeset**/**odeget**
  - New wrapper to mimic **ode15s**

Longer term TODO:

- Implement a MATLAB compatible version of **deval**
- Better handling of the options (avoid so much code repetition)