odeToJava: A problem-solving environment for initial-value problems

Andrew Kroshko

Department of Computer Science
University of Saskatchewan

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Introduction

`odeToJava`

- is a problem-solving environment (PSE) for research into numerical methods for initial-value problems (IVPs) in ordinary differential equations (ODEs)
- implements a broad range of numerical methods
- can provide numerical analysts with fine-grained control over the solution process
- allows composition of the different components of ODE software using modules

ODEs/IVPs

$$\frac{d\mathbf{y}}{dt}(t) = \mathbf{f}(t, \mathbf{y}(t))$$

- only has derivatives with respect to independent variable t
- independent variable is not always time
- $\mathbf{y}(t)$ is a vector of dependent variables
- an initial condition is given at t_0

$$\mathbf{y}(t_0) = \mathbf{y}_0$$

- not the only way to specify problem data (i.e., boundary-value problems)

Scientific problems described by ODEs

$$\frac{dv}{dt} = u$$
$$\frac{du}{dt} = \epsilon(1 - v^2)\frac{dv}{dt} - v, \quad \epsilon > 0$$

- Newtonian physics
- chemical reactions
- electronic circuits with capacitors, resistors, and inductors, etc.
- biological reactions and electrical activity
- population dynamics

ODEs to study or simulate other problems

- "method of lines" for simulation of PDEs
- as a component of larger simulation, e.g., chemical reaction in a fluid flow
- creating reduced models to study the dynamics of more complex problems

Requirement for numerical solvers

- only certain ODE systems have analytic solutions
  e.g., linear ODEs with constant coefficients
- solutions to most ODEs must be approximated
- even linear constant-coefficient ODEs are often more easily approximated than computed "exactly"!
- in practice, numerical methods must be used

Conventional solvers using function calls

```
 SUBROUTINE RODAS(N,FCN,IFCN,X,Y,XEND,H,
&                  RTOL,ATOL,ITOL,
&                  JAC,IJAC,MLJAC,MUJAC,DFX,IDFX,
&                  MAS,IMAS,MLMAS,MUMAS,
&                  SOLOUT,IOUT,
&                  WORK,LWORK,IWORK,LIWORK,RPAR,IPAR,IDID)
```

- system languages like FORTRAN and C/C++ widespread
- interface is function call with fixed signature
- take RHS function and limited number of parameters
- return the solution at final time
- return limited set of other data
- do not generally provide other software infrastructure

Problem-solving environments

- provide computational facilities for a target class of problems
- are productivity-oriented software that solves problems in ways familiar to researchers
- use terminology and methodology of the target class of problems
- limit specialized knowledge required of the underlying computer hardware, software, and algorithms
- provide facilities for easily post-processing, visualization, and performing further computations

ODE Solvers in MATLAB and similar PSEs

- similar to conventional solvers based on system languages
  - function call to invoke solvers
  - monolithic ODE solvers
  - limited amount of data returned
- scripting languages make computations simpler
  - more sophisticated data structures
  - straightforward integration of disparate functionality
  - additional mathematics, output, and visualization
  - extensive boilerplate code not required
  - automatic memory management
  - ideal for information handling and interfacing

Targeted or research-oriented PSEs

- some PSE research has been targeted towards IVPs
  - make it easier to solve IVPs (existing software is complex)
  - give researchers additional facilities to conduct their work
- types
  - expert systems to help end-users, Kamel, Ma, and Enright (1993)
  - GUI-based systems to assist researchers, Petcu and Dragan (2000)
  - object-oriented systems that accommodate many methods, Olsson (1997)
  - web-based or GUI-based systems for educational use, CODEE (Community of ODE educators)

Issues with contemporary scientific software

- future PSEs must solve issues related to scientific software development
- common difficulties with scientific software development
  - increasing reliance on and necessity for computer software
  - researchers lack skills of professional software developers
  - standard tools and methodologies unsuited to scientists
  - individual scientific codes often unique to a research group
  - increasingly complex computations and larger datasets
  - difficulty with documentation and understanding
  - increasingly complex post-processing and analysis
  - difficulties with verification and errors
  - difficulties in structuring code
- Nature article, Merali (2010)

The origin of the software "crisis"

- assumptions shown to be incorrect
  - information systems could be engineered conventionally
  - well-established engineering practices could be used
  - software process could be rigorously planned *a priori*
- Barbara Liskov: Programming the Turing Machine `https://www.youtube.com/watch?v=ibRar7sWulM`
  - military had difficulties with software for missiles and avionics
  - focus on hardware although sufficient for contemporary needs
  - many of the applications were well-understood
- NATO conference on software engineering, Naur and Randell (1968/1969)
- IBM OS development indicated experienced programmer can only produce 1000 lines/year, Brooks (1978)

Solutions to the software “crisis”

- code must allow reasoning to happen locally
- goto statement considered harmful; Dijkstra (1968)
- structured programming; Dahl, Dijkstra, and Hoare (1972)
- global variables considered harmful; Wulf and Shaw (1973)
- buy, don’t build; Brooks (1987)
- design patterns
- targeted languages and platforms
- improved tools, testing, and overall process
- open source

Similarities between contemporary issues in scientific software and software "crisis"

- development process and counter-intuitive limitations not taken into account during planning of software
- better methodologies for scientific software not identified
- increasing complexity means there exists difficulty creating adequate software
- focus on performance despite adequate computing power being available
- difficulties with maintainability, documentation, and general-purpose use
- optimal tools and training not determined

Additional issues

- *ad hoc* solutions for specific scientific problems common
- many basic results typically demonstrated in a few thousand lines of straightforward FORTRAN or C
- modern software and design techniques have not tended to help up until this point; Arge, Bruaset, and Langtangen (1999)
- lack of software to capture more complex computational needs and workflows
- managing both additional resources and resource limitations requires more complex software

Mathematical demonstrations

- term used by Söderlind and Wang (2006)
- computation that indicates analysis is correct
- not empirically rigorous
- identified as inadequate to design optimal adaptive methods
- Söderlind indicates a standard test protocol is required
- better software methodologies required to implement it

Purpose of odeToJava

- limitations to the number and scope of numerical studies
- each numerical study often results in a unique codebase
- there are >5400 journal articles in category 65L05 (numerical analysis of initial value problems) on MathSciNet
- many of these articles describe new methods
- other new IVP methods may exist in other categories or fields
- very few have been tested extensively, compared extensively, or have been used seriously in software

Purpose of odeToJava

- give numerical analysts finer-grained control
- common evaluations may not be adequate or useful
  - based on constant stepsize methods
  - analysis can be limited for combinations of numerical methods
  - assumptions used in mathematical analysis may break down
  - practical IVP software has many additional considerations

Purpose of odeToJava

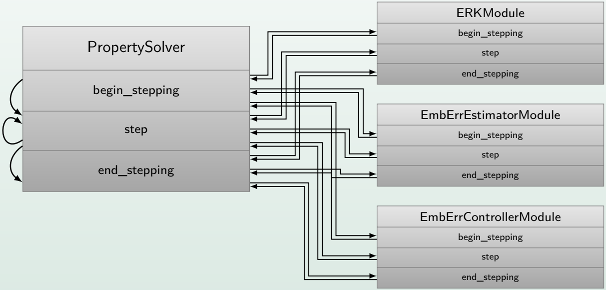
- JAVA a proven software platform
  - widely-used in business and web computing
  - software development tools
  - object-oriented
  - interface building
  - scalable
- share code between all methods as much as possible
- minimal new code required to experiment with new methods
- method- and experiment-specific code easy to reason about
- provide facilities to construct interfaces for an end-user

Libraries and Overall Structure

odeToJava
JScience/Javolution
Java/Java API
Java Virtual Machine

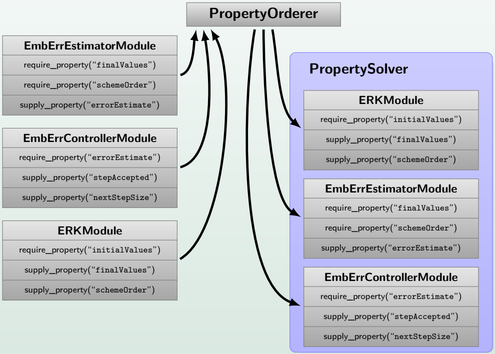
- JAVOLUTION contains high-performance data structures
- JSCIENCE has a linear algebra library and other scientific code

Modular solver



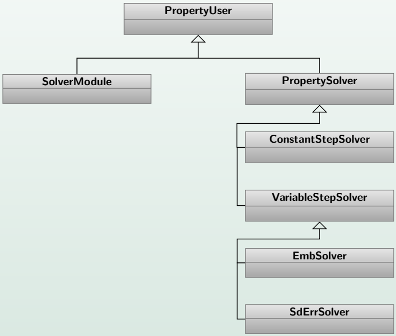
- promotes decoupling between components of an IVP solver
- global data structure is in `PropertySolver`
- uses mediator and pipeline patterns

Modular solver



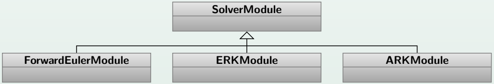
- automatic ordering of modules based on "properties"
- allows building solver by selecting a list of modules
- hides details of implementation

Modular solver



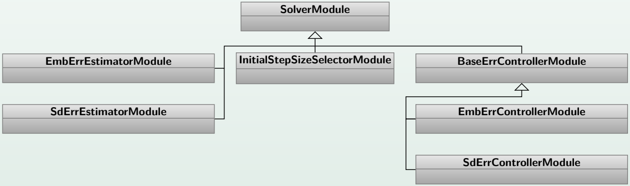
- different types of solvers for flow control
- modular design and decoupling
- allows a small number of solvers to work for most methods

Integration formula modules



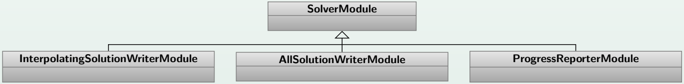
- many methods easily implemented
  - standard methods
  - experimental methods
  - problem-specific methods

Error control modules



- common adaptive schemes easily implemented
  - embedded error-estimation
  - step-doubling error-estimation
  - step-control based on error estimates
  - study adaptivity rigorously, Söderlind and Wang (2006)

Modular solver



- common output methods easily implemented
  - different output formats
  - monitoring
  - user interface
  - special formats required for post-processing

Automated running of experiments

- `IVPController`, `Testable`, `SolutionTester` classes
- straightforward selection of
  - integration method
  - solver type
  - initial stepsize
  - tolerances
- designed to be the “model” in a model-view-controller
- can replicate interface to many existing solvers
- easily allows components to be exchanged
- common framework allows rigorous testing
- minimal code changes required to test different methods
- reference solution input and solution output are text files

Test sets and ARK methods

- nonstiff DE set; Hull, Enright, *et al.* (1972)
- stiff DE test set; Enright *et al.* (1975)
- total of 60 problems with many different properties
- well-studied, most current is Enright and Pryce (1987)
- `odeToJava` uses a wide variety of ERK methods and ARK methods with Jacobian-based splitting
- showed widespread adoption of Dormand–Prince 5(4) is well-justified for non-stiff problems
- showed there is no one dominant ARK method

ERK methods

$$\mathbf{k}_i = \mathbf{f}\left(t_n + \Delta t_n c_i, \quad \mathbf{y}_n + \Delta t_n \sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j\right), \quad i = 1, 2, \ldots, s,$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta t_n \sum_{i=1}^{s} b_i \mathbf{k}_i,$$

- low cost per step
- suitable for non-stiff problems
- not suitable for stiff problems

ARK methods

$$\mathbf{f}(t, \mathbf{y}) = \sum_{\nu=1}^{N} \mathbf{f}^{[\nu]}(t, \mathbf{y}).$$

$$\mathbf{k}_i^{[1]} = \mathbf{f}^{[1]}\left(t_n + \Delta t_n c_i^{[1]}, \mathbf{y}_n + \Delta t_n \sum_{j=1}^{i-1}\left(a_{ij}^{[1]}\mathbf{k}_j^{[1]} + a_{ij}^{[2]}\mathbf{k}_j^{[2]}\right)\right), \quad i = 1, 2, \ldots, s,$$

$$\left(\mathbf{I} - \Delta t\, a_{ii}^{[2]}\mathbf{J}\right)\mathbf{k}_i^{[2]} = \mathbf{f}^{[2]}\left(t_n + \Delta t_n c_i^{[2]}, \mathbf{y}_n + \Delta t_n \sum_{j=1}^{i-1}\left(a_{ij}^{[1]}\mathbf{k}_j^{[1]} + a_{ij}^{[2]}\mathbf{k}_j^{[2]}\right)\right), \quad i = 1, 2, \ldots, s,$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta t_n \sum_{i=1}^{s}\left(b_i^{[1]}\mathbf{k}_i^{[1]} + b_i^{[2]}\mathbf{k}_i^{[2]}\right),$$

- one matrix factorization per stage (or per step)
- stiff linear component and nonstiff non-linear component
- Ascher, Ruuth, and Spiteri (1997); Kennedy and Carpenter (2003)

Arenstorf orbit problem

- 3-body problem of the Earth, moon, and a massless satellite
- satellite passes close to singularity at position of moon
- Hamiltonian problem that can be solved by symplectic methods that conserve momentum and nearly conserve energy
- considered ideal problem for variable-stepsize symplectic methods; Leimkuhler and Reich (2004)

Arenstorf orbit problem

$$H(\mathbf{q},\mathbf{p}) = \frac{p_1^2 + p_2^2}{2} - q_1 p_2 + q_2 p_1 - \frac{\mu}{\sqrt{(q_1 - \mu')^2 + {q_2}^2}} - \frac{\mu'}{\sqrt{(q_1 + \mu)^2 + q_2^2}},$$

$$\dot{\mathbf{q}} = \nabla H_{\mathbf{p}}(\mathbf{q},\mathbf{p}) = \begin{bmatrix} p_1 + q_2 \\ p_2 - q_1 \end{bmatrix},$$

$$\dot{\mathbf{p}} = -\nabla H_{\mathbf{q}}(\mathbf{q},\mathbf{p}) = -\begin{bmatrix} -p_2 + \frac{\mu'(q_1+\mu)}{((q_1+\mu)^2+{q_2}^2)^{3/2}} + \frac{\mu(q_1-\mu')}{((q_1-\mu')^2+{q_2}^2)^{3/2}} \\ p_1 + \frac{\mu' q_2}{((q_1+\mu)^2+{q_2}^2)^{3/2}} + \frac{\mu\, q_2}{((q_1-\mu')^2+{q_2}^2)^{3/2}} \end{bmatrix},$$

Störmer–Verlet method

$$
\begin{aligned}
\mathbf{p}_{n+\frac{1}{2}} &= \mathbf{p}_n - \frac{\Delta t}{2}\nabla_{\mathbf{q}} H(\mathbf{q}_n, \mathbf{p}_{n+\frac{1}{2}}),\\
\mathbf{q}_{n+1} &= \mathbf{q}_n + \frac{\Delta t}{2}\nabla_{\mathbf{p}} H(\mathbf{q}_n, \mathbf{p}_{n+\frac{1}{2}}) + \frac{\Delta t}{2}\nabla_{\mathbf{p}} H(\mathbf{q}_{n+1}, \mathbf{p}_{n+\frac{1}{2}}),\\
\mathbf{p}_{n+1} &= \mathbf{p}_{n+\frac{1}{2}} - \frac{\Delta t}{2}\nabla_{\mathbf{q}} H(\mathbf{q}_{n+1}, \mathbf{p}_{n+\frac{1}{2}})
\end{aligned}
$$

- second-order explicit method
- symplectic for Hamiltonian problems

Variable-stepsize symplectic methods

$$Q(\mathbf{q},\mathbf{p}) = \left(\frac{d_1 d_2}{v}\right)^{-\frac{\alpha}{2}},$$

$$G(\mathbf{q},\mathbf{p}) = \alpha\left[\frac{v_1}{v^2}\left(\frac{\mu'(q_1+\mu)}{d_1}+\frac{\mu(q_1-\mu')}{d_2}\right) - v_1\left(\frac{q_1+\mu}{d_1}+\frac{q_1-\mu'}{d_2}\right)\right.$$
$$\left. + \frac{v_2 q_2}{v^2}\left(\frac{\mu'}{d_1}+\frac{\mu}{d_2}\right) - q_2\left(\frac{1}{d_1}+\frac{1}{d_2}\right) - \frac{p_1 v_2 - p_2 v_1}{v^2}\right],$$

$$v_1 = p_1 + q_2, \qquad v_2 = p_2 - q_1, \qquad v^2 = {v_1}^2 + {v_2}^2,$$
$$d_1 = (q_1+\mu)^2 + q_2^2, \qquad d_2 = (q_1-\mu')^2 + q_2^2,$$

- based on Hairer and Söderlind (2005)
- conventional step controllers using heuristic methods cannot be applied to symplectic methods
- stepsize control based on a function of system state
- integrating step control

Variable-stepsize symplectic methods

$$\rho_{n+\frac{1}{2}} = \rho_n + \epsilon\, G(\mathbf{q}_n, \mathbf{p}_n)/2,$$

$$\mathbf{M} = \frac{1}{1 + \frac{\epsilon/\rho_{n+\frac{1}{2}}}{4}^2} \begin{bmatrix} 1 & \frac{\epsilon/\rho_{n+\frac{1}{2}}}{2} \\ -\frac{\epsilon/\rho_{n+\frac{1}{2}}}{2} & 1 \end{bmatrix},$$

$$\mathbf{p}_{n+\frac{1}{2}} = \mathbf{M}\left(\mathbf{p}_n - \frac{\epsilon/\rho_{n+\frac{1}{2}}}{2}\begin{bmatrix} \frac{\mu'(q_{1,n}+\mu)}{((q_{1,n}+\mu)^2+q_{2,n}{}^2)^{3/2}} + \frac{\mu(q_{1,n}-\mu')}{((q_{1,n}-\mu')^2+q_{2,n}{}^2)^{3/2}} \\ \frac{\mu' q_{2,n}}{((q_{1,n}+\mu)^2+q_{2,n}{}^2)^{3/2}} + \frac{\mu\, q_{2,n}}{((q_{1,n}-\mu')^2+q_{2,n}{}^2)^{3/2}} \end{bmatrix}\right),$$

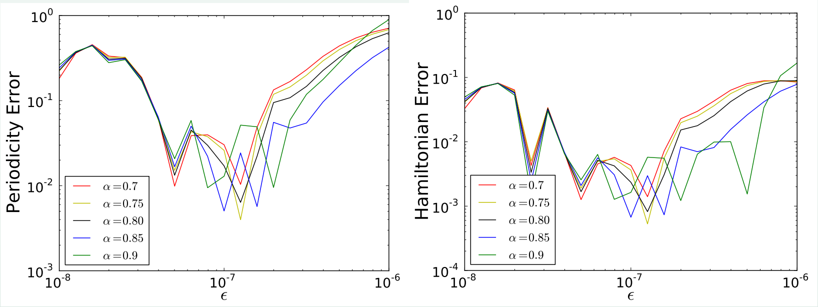
$$\mathbf{q}_{n+1} = \mathbf{M}\left(\mathbf{q}_n + \frac{\epsilon/\rho_{n+\frac{1}{2}}}{2}\begin{bmatrix} 2p_{1,n+\frac{1}{2}} + q_{n,2} \\ 2p_{2,n+\frac{1}{2}} - q_{n,1} \end{bmatrix}\right),$$

$$\mathbf{p}_{n+1} = \mathbf{p}_{n+\frac{1}{2}} - \frac{\epsilon/\rho_{n+\frac{1}{2}}}{2}\begin{bmatrix} -p_{2,n+\frac{1}{2}} + \frac{\mu'(q_{1,n+1}+\mu)}{((q_{1,n+1}+\mu)^2+q_{2,n+1}{}^2)^{3/2}} + \frac{\mu(q_{1,n+1}-\mu')}{((q_{1,n+1}-\mu')^2+q_{2,n+1}{}^2)^{3/2}} \\ p_{1,n+\frac{1}{2}} + \frac{\mu' q_{2,n+1}}{((q_{1,n+1}+\mu)^2+q_{2,n+1}{}^2)^{3/2}} + \frac{\mu\, q_{2,n+1}}{((q_{1,n+1}-\mu')^2+q_{2,n+1}{}^2)^{3/2}} \end{bmatrix},$$

$$\rho_{n+1} = \rho_{n+\frac{1}{2}} + \epsilon\, G(\mathbf{q}_{n+1}, \mathbf{p}_{n+1})/2,$$

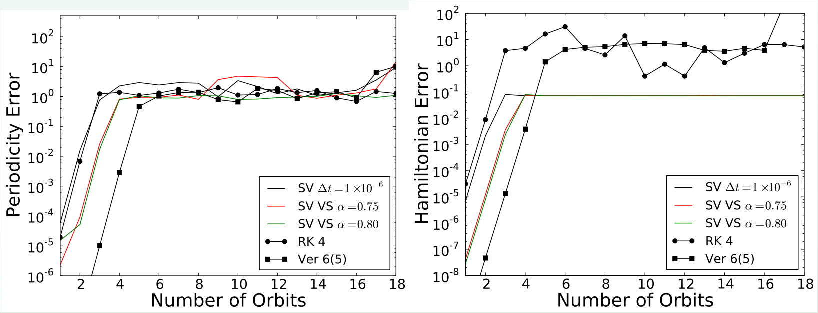
$$t_{n+1} = t_n + \epsilon/\rho_{n+\frac{1}{2}}.$$

Variable-stepsize symplectic methods



- there exists an optimum value of epsilon

Variable-stepsize symplectic methods



- variable-stepsize Störmer–Verlet has lowest error for some parameter values

OO programming and its limitations

- OO programming allows creation of a modular ODE solver
- limitations to OO programming
  - Liskov Substitution Principle limits utility of subtyping; Liskov and Wang (1994)
  - difficult to determine best abstractions and interfaces
  - optimal OO design often different from how humans think
  - allows APIs to become large and complex
  - high-quality OO software is labour-intensive
  - often has counter-intuitive restrictions on versatility

Use of JAVA in scientific computing

- most popular in first 5 years of 21st century
- many C libraries were ported to JAVA
  - `Colt` includes bindings to `BLAS` and `LAPACK`
- used in GUI code for MATLAB and many other PSEs
- used by CERN and other large deployments
- contemporary interest because of scalability and robustness

Advantages of JAVA

- most popular programming language in industry
- integrates well with internet and web
- highly scaleable
- many well-developed tools for large code bases
  - highly automated development possible
  - automated navigation and understanding of code
  - packaging and deployment

Disadvantages of JAVA

- tends to be very verbose with a lot of boilerplate code
- type system can be too restrictive
- can require domain-specific languages or complex interfaces for flexible applications
- difficulty interfacing with other platforms
- floating-point arithmetic not tested as extensively as more well-established scientific platforms

Conclusions

- demonstrated a universal and modular IVP solver is possible
- has advantage of only one codebase
- demonstrated method and problem combinations that have not been widely tested
- software techniques learned can be applied to more complex classes of problems

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