Robust time integration methods - Emil Constantinescu
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- Algorithms to solve ODEs, DAEs, PDEs: $y'(t) = f(t, y(t)),\, t_0 \leq t \leq T,\, y(t_0) = y_0$
- Time stepping algorithms: Runge-Kutta, linear multistep, general linear schemes
- Partitioned methods for particular systems: Implicit-Explicit (IMEX or semi-implicit), multirate (resolve multiple scales)
- No one-method-fits-all, need to consider problem characteristics (stiffness, conservation, smoothness, geometry), computational architecture
- Optimize methods: <u>stability</u> and <u>accuracy</u>
- Augment schemes with error estimators, step controllers, predictors, preconditioners
- Implementation in PETSc library

Accuracy:

- Problem: $y'(t) = f(t, y(t))$

elementary derivatives:

$$y' = f$$
$$y'' = f'f$$
$$y^{(3)} = f''(f,f) + f'f'f$$
$$\dots$$

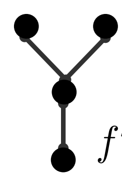
- E.g., Runge-Kutta: $y_{n+1} = \quad y_n + \Delta t \sum_{i=1}^{s} b_i f\left(Y_i\right)$

$\Psi($$) = R(a,b)$

$$Y_i = \quad y_n + \Delta t \sum_{j=1}^{i-1} a_{ij} f\left(Y_j\right)$$

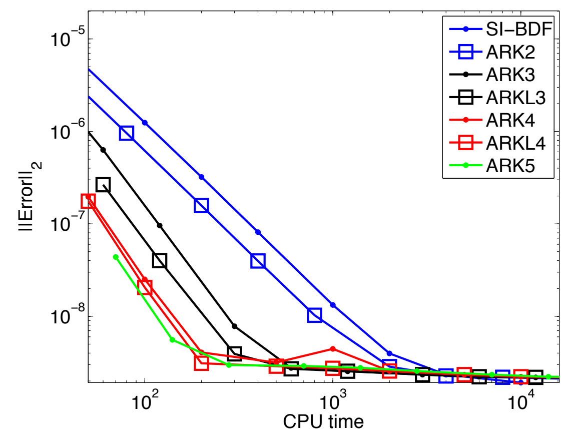
- Order conditions: $\sum_i b_i = 1\,, \; \sum_{ij} b_i a_{ij} = \frac{1}{2}\,, \dots$

- Order conditions “form” a noncommutative algebraic group:



$f'f''(f,f)$

- High order methods are typically more robust



- Perturbed asymptotic expansions may be needed

Hopf algebras, Feynman graphs, and renormalization: Brouder C. (2000) Runge–Kutta methods and renormalization. *Eur. Phys. J. C.*, 12, 521–534

Symplecticity:

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

- Condition: $b_i a_{ij} + b_j a_{ji} = b_i b_j$

  Problem: $\ddot{q} = f(q)$

  Störmer-Verlet:
$$p_{n+1/2} = p_n + \frac{\Delta t}{2} f(q_n)$$
$$q_{n+1} = q_n + \Delta t p_{n+1/2}$$
$$p_{n+1} = p_{n+1/2} + \frac{\Delta t}{2} f(q_{n+1})$$

Störmer-Verlet as Runge-Kutta

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

$$\{q,p\}_{[n+1]} = e^{\frac{1}{2}\Delta t f(.)} e^{\Delta t p} e^{\frac{1}{2}\Delta t f(.)} \{q,p\}_{[n]}$$

Stability:

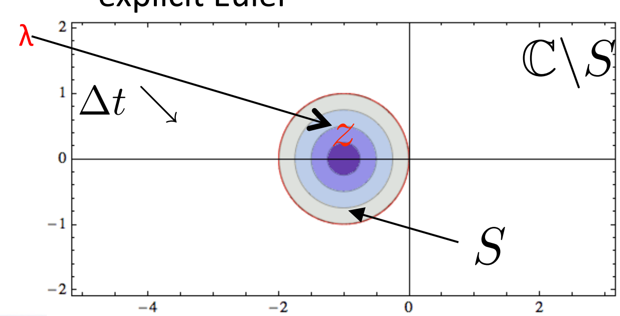
- Consider the IVP: $y'(t) = F(t, y(t)),\ t_0 \le t \le T,\ y(t_0) = y_0$

$$\lambda = \text{eig}\left(\frac{\partial F}{\partial y}\right)$$

- Linear stability analysis: $y' = \lambda y\,, \quad y_{n+1} = R(\lambda \Delta t) y_n\,, \quad S = \{z \in \mathbb{C};\ |R(z)| \le 1\}$

- E.g., forward Euler: $y_{n+1} = \underbrace{(1 + \lambda \Delta t)}_{R(z)=1+z} y_n$

explicit Euler



Optimal methods

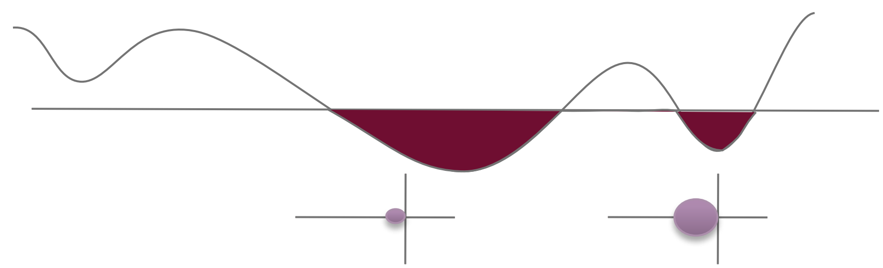
- Formulate the method design as a mathematical programming problem: search for the **global optimum** set of coefficients that define the search criteria: nonlinear multiobjective optimization problem:

$$\min_{a,b,c,\ldots} \overbrace{\Lambda\left(1-\gamma(\mathcal{T}_e)\sum b_i\,\Psi(\mathcal{T}_e)\right)}^{\text{Error}} + \overbrace{\|\beta_s(\lambda,\mu)\|}^{\text{Stability}}\,, \qquad r(\mathcal{T}_e)=p+1$$

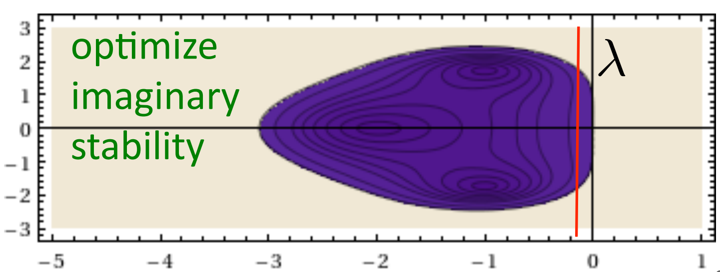
$$\text{subject to } \sum b_j\Psi(\mathcal{T}_p)=1/\gamma(\mathcal{T}_p)$$

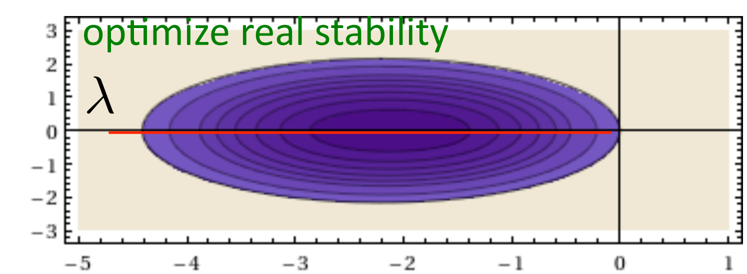
$$|R(\alpha_E\lambda\Delta t)|\le 1\,,\;\; \lambda\in[-\beta_S,0]$$

- Global optimization [BARON] allows construction of families of methods – Pareto surface



- Stability region (SR) leads to a **semi-infinite program**: $\max_{|R(\gamma\lambda,\varepsilon)|\le 1,\,\forall\gamma\in[0,\beta]} \beta$

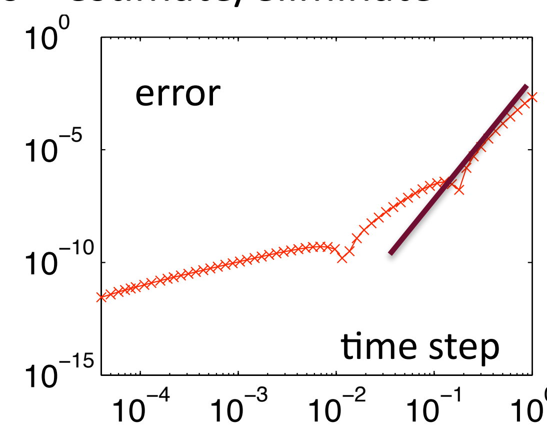




Final remarks

1. Perform stability analysis to obtain algebraic constraints – how large the time step can be, augmented criterion that includes the acceptance rate and force calculation costs == [Balint et al.] limits have been identified, more d.o.f. may provide relief.

2. Analyze stiffness effects by perturbed expansion analyses – estimate/eliminate large error constants and stability issues



3. Develop time adaptivity by using reversible step size controllers – reduce computational cost. Controller/error estimators are inexpensive == experiments exhibited a loss of symplectic properties. Identify and solve the problem.

4. Use all this machinery to develop new optimal methods via global optimization algorithms and implement in Chroma/PETSc.