A new approach to control the global error of numerical methods for ODEs

(SciCADE 2011 presentation)

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- Introduction to Double Quasi-Consistency.

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- Fixed-Stepsize Doubly Quasi-Consistent EPP Methods.

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- Variable-Stepsize EPP Methods of Interpolation Type.
- Efficient Global Error Estimation and Control.

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- Global Error Estimation and Control.
- Variable-Stepsize EPP Methods of Interpolation Type.
- Efficient Global Error Estimation and Control.
- Conclusion.

Double Quasi-Consistency

In this paper, we consider ODE of the form

$$x'(t) = g\big(t, x(t)\big), \quad t \in [t_0, t_{end}], \quad x(0) = x^0 \qquad (1)$$

where $x(t) \in \mathbb{R}^m$ and $g : D \subset \mathbb{R}^{m+1} \longrightarrow \mathbb{R}^m$.
We assume:

- the right-hand side of ODE (1) is sufficiently smooth;

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where $x(t) \in \mathbb{R}^m$ and $g : D \subset \mathbb{R}^{m+1} \rightarrow \mathbb{R}^m$.
We assume:

- the right-hand side of ODE (1) is sufficiently smooth;
- there exists a unique solution $x(t)$ to equation (1) on the interval $[t_0, t_{end}]$.

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Can we do better ?

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- However, Global Error Control can be very expensive and requires several numerical solutions over the integration interval [Skeel, 1986, 1989].

Can we do better ?

- More precisely, can we control the global error for one integration ?

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- Thus, it is clear that if we want to control the global error effectively (i.e. for one integration) we must not control it. This sounds contradictory.

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- Thus, it is clear that if we want to control the global error effectively (i.e. for one integration) we must not control it. This sounds contradictory.

Who (or what) will control the global error ?

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- More precisely, we control the local error. This can be done efficiently.
- The method ensures that True Error $\approx$ Local Error at any grid point.
- More formally, numerical schemes of order s considered here satisfy *(τ_k is a size of the k-th step)*

$$\text{True Error}(k+1) = \text{Local Error}(k+1) + \mathcal{O}(\tau_k^{s+1}). \quad (2)$$

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- The methods considered in this paper belong to the class of quasi-consistent schemes because the orders of their local and global errors with respect to stepsize coincide.
- Moreover, we require additionally that the principal terms of the local and global errors coincide, i.e. these errors are asymptotically equal.

That is why the usual local error control is expected to produce automatically numerical solutions satisfying user-supplied accuracy requirements for one integration.

Double Quasi-Consistency

Methods satisfying condition (2):

$$\text{True Error}(k+1) = \text{Local Error}(k+1) + \mathcal{O}(\tau_k^{s+1}), \qquad (2)$$

are further refereed to as Doubly Quasi-Consistent.

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HISTORY on Quasi-Consistent Integration:

- Skeel discovered the property of quasi-consistency in 1976.
- Skeel and Jackson found the first quasi-consistent methods among fixed-stepsize Nordsieck formulas in 1977.
- Kulikov and Shindin proved in 2006 that conventional Nordsieck formulas cannot exhibit the quasi-consistent behaviour on variable meshes because of the order reduction phenomenon.

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HISTORY on Quasi-Consistent Integration (cont.):

- In 2009, Weiner et al. constructed actual variable-stepsize quasi-consistent numerical schemes in the family of explicit two-step peer formulas.
- Kulikov proved in the same year that there exists no doubly quasi-consistent Nordsieck formula.

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Further, we prove Existence of Doubly Quasi-Consistent Numerical Schemes in the family of fixed-stepsize s-stage Explicit Parallel Peer methods (EPP-methods)

Fixed-Stepsize EPP Methods

We deal further with numerical schemes of the form

$$x_{ki} = \sum_{j=1}^{s} b_{ij} x_{k-1,j} + \tau \sum_{j=1}^{s} a_{ij} g(t_{k-1,j}, x_{k-1,j}), \qquad (3)$$

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$i = 1, 2, \ldots, s$, or in the matrix form

$$X_k = (B \otimes I_m) X_{k-1} + \tau (A \otimes I_m) g(T_{k-1}, X_{k-1})$$

where

$$T_k := (t_{ki})_{i=1}^{s}, \; X_k := (x_{ki})_{i=1}^{s}, \; g(T_k, X_k) := g(t_{ki}, x_{ki})_{i=1}^{s},$$

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DEFINITION 1: The peer method (3) is consistent of *order* p if and only if the following order conditions hold:

$$\mathcal{AB}_i(l) := c_i^l - \sum_{j=1}^{s}\Big(b_{ij}(c_j-1)^l + l\, a_{ij}(c_j-1)^{l-1}\Big) = 0,\ \ l \le p.$$

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THEOREM 1: The peer method (3) of order p is doubly quasi-consistent if and only if its coefficients a_{ij}, b_{ij} and c_i satisfy the following conditions:

$$\mathcal{AB}(l) = 0, \quad l = 0, 1, \ldots, p-1,$$

$$B \cdot \mathcal{AB}(p) = 0,\ \ B \cdot \mathcal{AB}(p+1) = 0,\ \ A \cdot \mathcal{AB}(p) = 0.$$

Fixed-Stepsize EPP Methods

With the use of Theorem 1, we yield the following doubly quasi-consistent EPP-method (3) presented by its coefficients:

$$A = \begin{pmatrix} \frac{89}{144} & \frac{23}{48} & -\frac{5}{36} \\ -\frac{133}{144} & \frac{29}{48} & \frac{55}{36} \\ -\frac{37}{144} & \frac{41}{48} & \frac{10}{9} \end{pmatrix},$$

$$B = \begin{pmatrix} \frac{11}{18} & \frac{1}{2} & -\frac{1}{9} \\ \frac{11}{18} & \frac{1}{2} & -\frac{1}{9} \\ \frac{11}{18} & \frac{1}{2} & -\frac{1}{9} \end{pmatrix}, \quad c = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \\ 1 \end{pmatrix}.$$

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This is a 3-stage explicit parallel peer method of order 2.

Global Error Estimation & Control

TRUE ERROR EVALUATION: Having used an embedded peer method (3) with coefficients A_{emb}, B_{emb} and c, we arrive at the error evaluation scheme of the form

$$\Delta_1 X_k = \big((B_{emb} - B) \otimes I_m\big) X_{k-1} + \tau\big((A_{emb} - A) \otimes I_m\big) g(T_{k-1}, X_{k-1}) \tag{4}$$

where $\Delta_1 X_k$ denotes the principal term of the true error of the doubly quasi-consistent peer method and X_{k-1} implies the numerical solution computed by the same peer method. The global error estimation formula (4) is cheap.

Global Error Estimation & Control

THEOREM 2: Let the peer method (3) be doubly quasi-consistent and of order p. Then formula (4) computes the principal term of its true error at grid points if and only if the coefficients A_{emb}, B_{emb} and c of the embedded peer method satisfy the following conditions:

$$\mathcal{AB}(l)_{emb} = 0,\ l = 0, 1, \ldots, p, \quad B_{emb} \cdot \mathcal{AB}(p) = 0$$

where the vectors $\mathcal{AB}(l)_{emb}$, $l = 0, 1, \ldots, p$, are calculated for the coefficients of the embedded formula (3) and the vector $\mathcal{AB}(p)$ is evaluated for the coefficients of the doubly quasi-consistent peer method in the embedded pair.

Global Error Estimation & Control

With the use of Theorem 2, the embedded peer method (3) for the doubly quasi-consistent peer scheme above is chosen to have the coefficients:

$$A_{emb} = \begin{pmatrix} -\frac{1}{18} & \frac{47}{96} & \frac{151}{288} \\ \frac{7}{18} & -\frac{35}{96} & \frac{341}{288} \\ \frac{58}{18} & -\frac{476}{96} & \frac{1069}{288} \end{pmatrix},$$

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This embedded formula is of classical order 2 and has the local error of $\mathcal{O}(\tau^3)$.

Global Error Estimation & Control

GLOBAL ERROR CONTROL ALGORITHM:

1. $k := 0$, $\tau := \tau_{int}$; ($\tau_{int}, \gamma \in (0,1)$ are set);
2. While $t_k < t_{end}$ do,

   $t_{k+1} := t_k + \tau$, compute X_{k+1}, $\Delta_1 X_{k+1}$;
3. If $\max_k \|\Delta_1 X_{k+1}\| > \epsilon_g$,

   then $\tau := \gamma\tau \left(\epsilon_g / \max_k \|\Delta_1 \tilde{X}_{k+1}\|\right)^{1/p}$, go to 1,

   else Stop.

Global Error Estimation & Control

TEST PROBLEM 1: Simple Problem

$$x_1'(t) = 2t x_2^{1/5}(t) x_4(t), \; x_2'(t) = 10t \exp\Big(5\big(x_3(t) - 1\big)\Big) x_4(t),$$

$$x_3'(t) = 2t x_4(t), \quad x_4'(t) = -2t \ln\big(x_1(t)\big),$$

where $t \in [0, 3]$, $x(0) = (1, 1, 1, 1)^T$.

Global Error Estimation & Control

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The exact solution is well-known:

$$x_1(t) = \exp\big(\sin t^2\big), \quad x_2(t) = \exp\big(5\sin t^2\big),$$

$$x_3(t) = \sin t^2 + 1, \quad x_4(t) = \cos t^2$$

Global Error Estimation & Control

TEST PROBLEM 2: Restricted Three Body Problem

$$x_1''(t) = x_1(t) + 2x_2'(t) - \mu_1 \frac{x_1(t) + \mu_2}{y_1(t)} - \mu_2 \frac{x_1(t) - \mu_1}{y_2(t)},$$

$$x_2''(t) = x_2(t) - 2x_1'(t) - \mu_1 \frac{x_2(t)}{y_1(t)} - \mu_2 \frac{x_2(t)}{y_2(t)},$$

$$y_1(t) = \Big((x_1(t) + \mu_2)^2 + x_2^2(t)\Big)^{3/2}, y_2(t) = \Big((x_1(t) - \mu_1)^2 + x_2^2(t)\Big)^{3/2}$$

where $t \in [0, T]$, $T = 17.0652165601579625588917$, $\mu_1 = 1 - \mu_2$ and $\mu_2 = 0.012277471$. The initial values are: $x_1(0) = 0.994$, $x_1'(0) = 0$, $x_2(0) = 0$, $x_2'(0) = -2.0015851063790825224$.

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Its solution-path is periodic.

Global Error Estimation & Control

NUMERICAL RESULTS for our Test Problems:

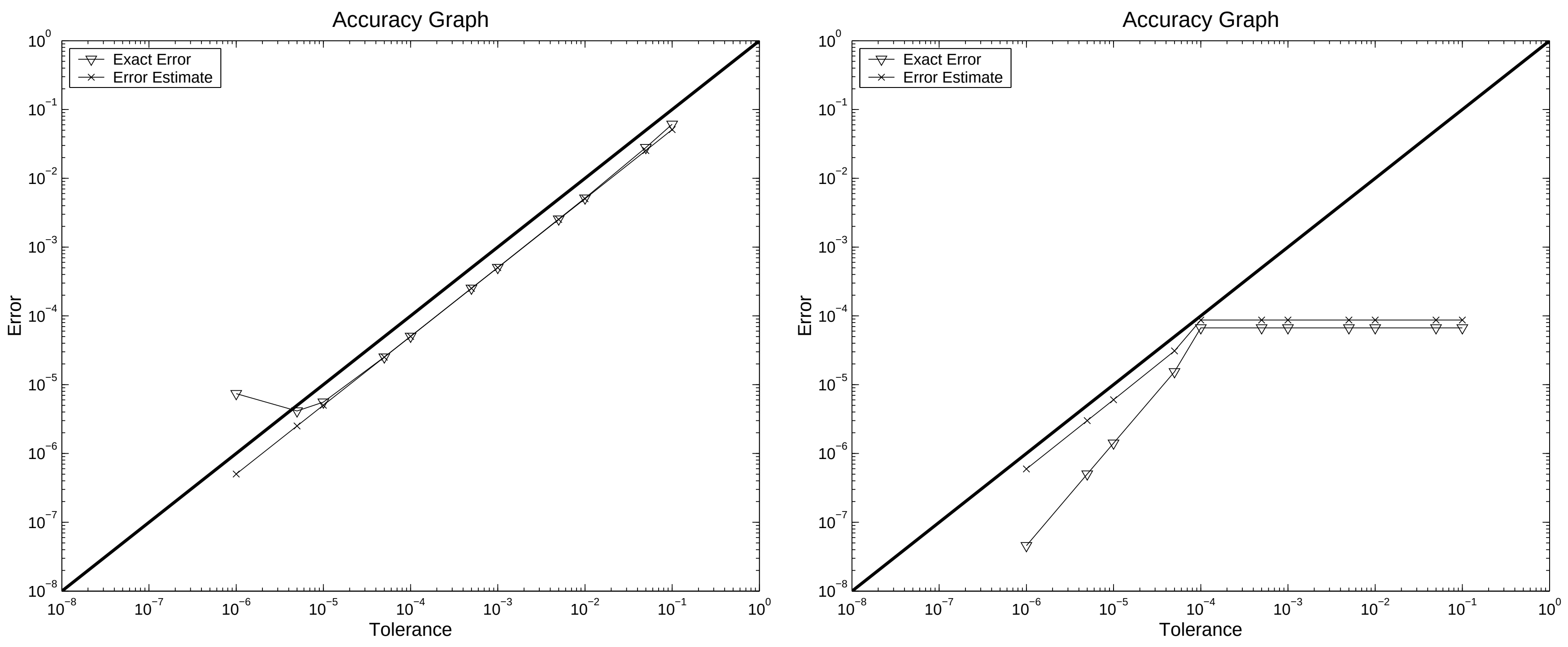

Figure 1. True and estimated errors of the doubly quasi-consistent peer method applied to the test problems.

Global Error Estimation & Control

DYNAMIC BEHAVIOUR OF THE ERRORS AND THE ESTIMATE:

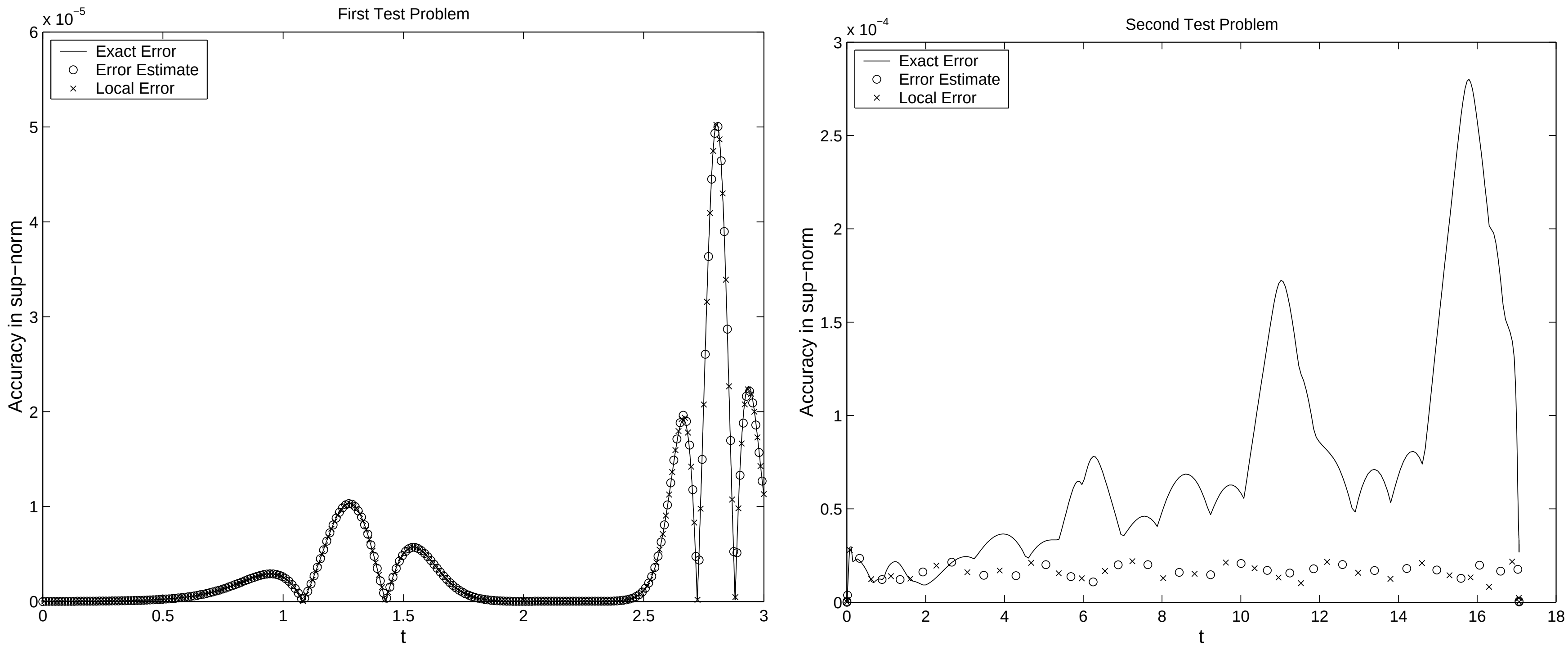

Figure 2. Numerical results obtained for the method when $\epsilon_g = 10^{-04}$.

Global Error Estimation & Control

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Accommodation of Doubly Quasi-Consistent Numerical Schemes to variable meshes

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The fixed-stepsize methods are not efficient!

Thus, the second issue is:
Accommodation of Doubly Quasi-Consistent Numerical Schemes to variable meshes

This is to be done on the basis of:
The Polynomial Interpolation Technique

EPP Methods of Interpolation Type

We introduce a variable grid with a diameter τ on the integration interval $[t_0, t_{end}]$ by

$$w_\tau := \{t_{k+1} = t_k + \tau_k,\ k = 0, 1, \ldots, K-1,\ t_K = t_{end}\}$$

where $\tau := \max_{0 \le k \le K-1}\{\tau_k\}$. It is clear that EPP-method (3) cannot be applied on w_τ.

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Let us consider that we have completed the $(k-1)$-th step of the size τ_{k-1} and computed the numerical solution $x_{k-1,i}^{k-1}$, $i = 1, 2, \ldots, s$. Further, we want to advance the next step of the size $\tau_{\mathbf{k}} \neq \tau_{\mathbf{k-1}}$.

EPP Methods of Interpolation Type

At this point, we need two auxiliary grids:

$$w_{k-1} := \{t_{k-1,i}^{k-1} = t_k + (c_i - 1)\tau_{k-1},\ i = 1, 2, \ldots, s\}$$

and

$$w_k := \{t_{k-1,i}^{k} = t_k + (c_i - 1)\tau_k,\ i = 1, 2, \ldots, s\}$$

where c_i, $i = 1, 2, \ldots, s$, are nodes of the fixed-stepsize EPP-method (3), which are considered to be distinct.

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where c_i, $i = 1, 2, \ldots, s$, are nodes of the fixed-stepsize EPP-method (3), which are considered to be distinct. Now we utilize the interpolating polynomial $\mathbf{H_{k-1}^{s-1}(t)}$ of degree $\mathbf{s-1}$ fitted to the data $\mathbf{x_{k-1,i}^{k-1}}$, $\mathbf{i = 1, 2, \ldots, s}$, from the most recent step to accommodate this numerical solution to the new stepsize $\tau_\mathbf{k}$.

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2. We compute the numerical solution $\mathbf{x^k_{ki}}$, $\mathbf{i = 1, 2, \ldots, s}$, for the next step of the size $\tau_\mathbf{k}$ by formula (3).

EPP Methods of Interpolation Type

DEFINITION 2: The EPP-method of the form

$$t_{k-1,j}^{k} = t_k + (c_j - 1)\tau_k, \quad x_{k-1,j}^{k} = H_{k-1}^{s-1}(t_{k-1,j}^{k}), \qquad (5a)$$

$$x_{ki}^{k} = \sum_{j=1}^{s} b_{ij} x_{k-1,j}^{k} + \tau_k \sum_{j=1}^{s} a_{ij} g(t_{k-1,j}^{k}, x_{k-1,j}^{k}), \qquad (5b)$$

where $H_{k-1}^{s-1}(t)$ is the interpolating polynomial of degree $s-1$ fitted to the numerical solution $x_{k-1,i}^{k-1}$, $i = 1, 2, \ldots, s$, from the previous step is called the *Explicit Parallel Peer method with polynomial interpolation of the numerical solution* (or, briefly, *the interpolating EPP-method*).

EPP Methods of Interpolation Type

THEOREM 3: Let the EPP-method (3) with distinct nodes c_i be zero-stable. Then the interpolating EPP-method (5) is zero-stable if and only if the following condition holds:

$$\left\| \prod_{l=0}^{m} BH(\theta_{k+m-l}) \right\| \leq R, \text{ for all } k \geq 0 \text{ and } m \geq 0 \qquad (6)$$

where $h_{ij}(\theta_k) := \prod_{\substack{n=1, \\ n \neq j}}^{s} \frac{(c_i - 1)\theta_k - c_n + 1}{c_j - c_n}, \quad i, j = 1, 2, \ldots, s,$

R is a finite constant and $\theta_k := \tau_k / \tau_{k-1}$ is the corresponding stepsize ratio of the grid w_τ.

EPP Methods of Interpolation Type

THEOREM 3: Let the EPP-method (3) with distinct nodes c_i be zero-stable. Then the interpolating EPP-method (5) is zero-stable if and only if the following condition holds:

$$\left\| \prod_{l=0}^{m} BH(\theta_{k+m-l}) \right\| \leq R, \text{ for all } k \geq 0 \text{ and } m \geq 0 \qquad (6)$$

where $h_{ij}(\theta_k) := \prod_{\substack{n=1,\\ n\neq j}}^{s} \frac{(c_i-1)\theta_k - c_n + 1}{c_j - c_n}, \quad i,j = 1,2,\ldots,s,$

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EPP Methods of Interpolation Type

DEFINITION 3: The set of grids where the interpolating EPP-method (5) is stable is further referred to as *the set* $\mathbb{W}^{\infty}_{\omega_1,\omega_2}(t_0, t_{end})$ *of admissible grids*. Such grids satisfy the condition

$$0 \le \omega_1 < \theta_k < \omega_2 \le \infty, \; k = 0, 1, ..., K-1, \tag{7}$$

with constants ω_1 and ω_2 for which $\omega_1 \le 1 \le \omega_2$.

EPP Methods of Interpolation Type

DEFINITION 4: The fixed-stepsize EPP-method (3) is said to be *strongly stable* if its propagation matrix B has only one simple eigenvalue at one and all others lie in the open unit disc.

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THEOREM 4: Let the underlying fixed-stepsize s-stage EPP-method (3) of consistency order $p \geq 0$ and with distinct nodes c_i be strongly stable. Then there exist constants ω_1 and ω_2, satisfying (7), such that the corresponding s-stage interpolating EPP-method (5) is stable on any grid from the set $\mathbb{W}^{\infty}_{\omega_1,\omega_2}(t_0, t_{end})$.

EPP Methods of Interpolation Type

DEFINITION 5: The fixed-stepsize EPP-method (3) is said to be *optimally stable* if its propagation matrix B has only one simple eigenvalue at one and all others are zero.

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THEOREM 5: Let the underlying fixed-stepsize s-stage EPP-method (3) with distinct nodes c_i be consistent of order $p \geq 0$. Suppose that its propagation matrix B satisfies

$$B = \mathbb{1} v^T \tag{8}$$

where $\mathbb{1} := (1, 1, \ldots, 1)^T$ and $v := (v_1, v_2, \ldots, v_s)^T$. Then the corresponding s-stage interpolating EPP-method (5) is stable on any grid from the set $\mathbb{W}^{\infty}_{0,\infty}(t_0, t_{end})$.

EPP Methods of Interpolation Type

THEOREM 6: Let the right-hand side of ODE (1) be $\max\{p, s-1\}$ times continuously differentiable in a neighborhood of the exact solution and the stable EPP-method (3) with distinct nodes c_i be consistent of order $p \geq 1$. Suppose that the starting vector X_0^0 is known with an error of $\mathcal{O}(\tau^{\min\{p,s-1\}})$ and there exists a nonempty set $\mathbb{W}^{\infty}_{\omega_1,\omega_2}(t_0, t_{end})$ of admissible grids with finite parameter ω_2. Then the EPP-method (5) is convergent of order $\min\{p, s-1\}$, i.e. its global error satisfies

$$\|X(T_k^k) - X_k^k\| \leq C\tau^{\min\{p,s-1\}}, \quad k = 1, 2, \ldots, K.$$

where C is a finite constant.

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EPP Methods of Interpolation Type

REMARK 1: Additionally, Theorem 6 says that **double quasi-consistency condition (2)** does not work in general to improve the convergence order of **interpolating EPP-methods (5)** because of the variable matrix $H(\theta_k)$ involved in numerical integration.

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Further, we discuss how to accommodate **double quasi-consistency** to error estimation in **interpolating EPP-methods**.

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Further, we discuss how to accommodate **double quasi-consistency** to error estimation in **interpolating EPP-methods**. We impose the following extra condition:

$$\tau/\tau_k \leq \Omega < \infty, \quad k = 0, 1, \ldots, K-1, \tag{9}$$

where τ is the diameter of the grid. The set of grids satisfying (7) and (9) is denoted by $\mathbb{W}^{\mathbf{\Omega}}_{\omega_1,\omega_2}(\mathbf{t_0}, \mathbf{t_{end}})$.

EPP Methods of Interpolation Type

THEOREM 7: Let ODE (1) be sufficiently smooth and the stable EPP-method (3) of order $p \geq 1$ and with distinct nodes c_i be doubly quasi-consistent. Suppose that another solution $\bar{X}_k^k$ of order $\min\{p+1, s\}$ is known for a mesh w_τ and the polynomial $H_{k-1}^{s-1}(t)$ satisfies

$$p \leq s - 1. \tag{10}$$

Then the interpolating EPP-method

$$X_k^k = (B \otimes I_m)\bar{H}_{k-1}^{s-1}(T_{k-1}^k) + \tau_k(A \otimes I_m)g(T_{k-1}^k, \bar{H}_{k-1}^{s-1}(T_{k-1}^k))$$

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EPP Methods of Interpolation Type

REMARK 2: If the more accurate numerical solution $\bar{\mathbf{X}}_{\mathbf{k}}^{\mathbf{k}}$ in the formulation of Theorem 7 is computed by another s-stage interpolating EPP-method (5) then condition (10) must be replaced with the more stringent one

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- Notice that utilization of another s-stage interpolating EPP-method (5) is a natural requirement of the embedded method error estimation presented by formula (4).

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- Notice that utilization of another s-stage interpolating EPP-method (5) is a natural requirement of the embedded method error estimation presented by formula (4).
- Thus, Remark 2 allows the same numerical solution $\bar{\mathbf{X}}_{\mathbf{k}}^{\mathbf{k}}$ to be used effectively in the doubly quasi-consistent method and in our error evaluation scheme as well.

Efficient Global Error Control

CONSTRUCTION of EMBEDDED INTERPOLATING EPP-METHODS:

- It follows from Theorem 7 and Remark 2 that the embedded s-stage underlying fixed-stepsize EPP-methods (3) must be of **consistency orders** $s-3$ and s.

Efficient Global Error Control

CONSTRUCTION of EMBEDDED INTERPOLATING EPP-METHODS:

- It follows from Theorem 7 and Remark 2 that the embedded s-stage underlying fixed-stepsize EPP-methods (3) must be of **consistency orders** $s-3$ and s.
- the lower order method is to be **doubly quasi-consistent of order** $s-2$ and, hence, it is convergent of the same order on equidistant meshes.

Efficient Global Error Control

CONSTRUCTION of EMBEDDED INTERPOLATING EPP-METHODS (cont.):

- We fit the interpolating polynomial to the numerical solution obtained from the higher order embedded formula and denote it further by $\bar{H}_{k-1}^{s-1}(t)$.

Efficient Global Error Control

CONSTRUCTION of EMBEDDED INTERPOLATING EPP-METHODS (cont.):

- We fit the interpolating polynomial to the numerical solution obtained from the higher order embedded formula and denote it further by $\bar{H}^{s-1}_{k-1}(t)$.
- Our error estimation formula is presented by

$$\Delta_1 X_k^k = \Big((B_{emb} - B) \otimes I_m\Big)\bar{X}^k_{k-1} + \\ + \tau_k\Big((A_{emb} - A) \otimes I_m\Big) g(T^k_{k-1}, \bar{X}^k_{k-1})$$

where A, B and A_{emb}, B_{emb} are coefficients of the EPP-methods of orders $s-2$ and $s-1$, respectively.

Efficient Global Error Control

- In this way, we derive three pairs of embedded interpolating EPP-methods of orders $s-2$ and $s-1$ abbreviated further as **IEPP23**, **IEPP34** and **IEPP45**.

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- All these numerical schemes satisfy the following conditions imposed on their coefficients:

$$B_{emb} = B = \mathbb{1}v^T \quad \text{and} \quad c_{emb} = c.$$

Thus, **IEPP23**, **IEPP34** and **IEPP45** are determine completely by fixing two matrices A, A_{emb} and two vectors c and v.

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Efficient Global Error Control

NUMERICAL RESULTS for our Test Problems:

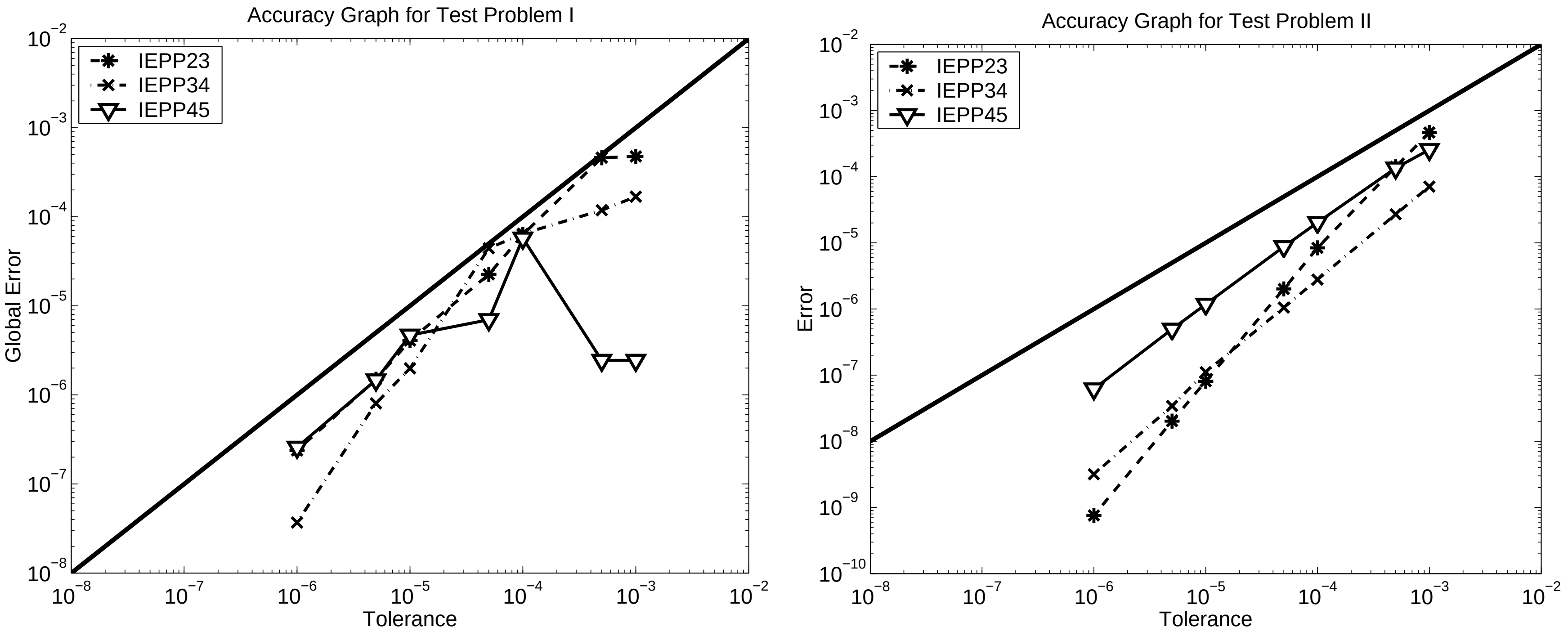

Figure 3. Exact errors of the embedded peer schemes with built-in our error estimation.

Efficient Global Error Control

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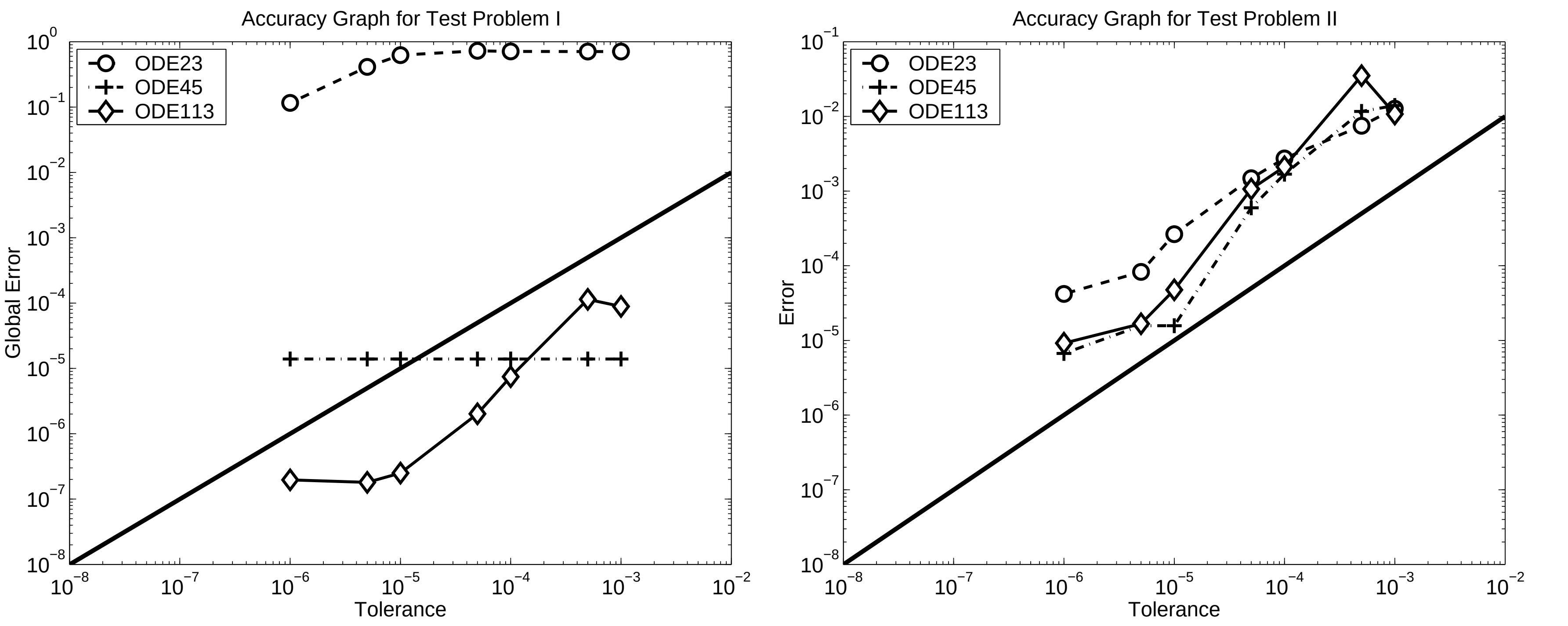

Figure 4. Exact errors of all explicit MatLab solvers with relative error control set by "RelTol"="AbsTol".

Efficient Global Error Control

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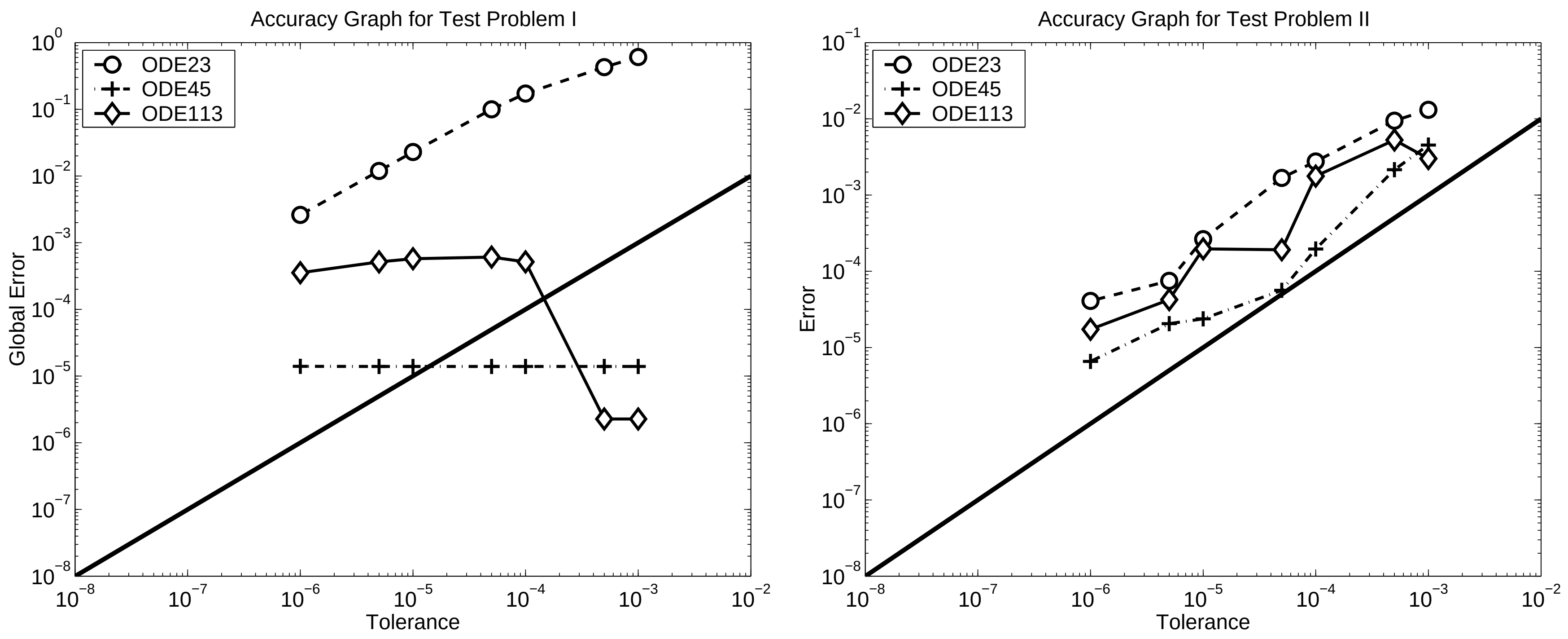

Figure 5. Exact errors of all explicit MatLab solvers without relative error control set by "RelTol"$:= 1.0E - 10$.

Efficient Global Error Control

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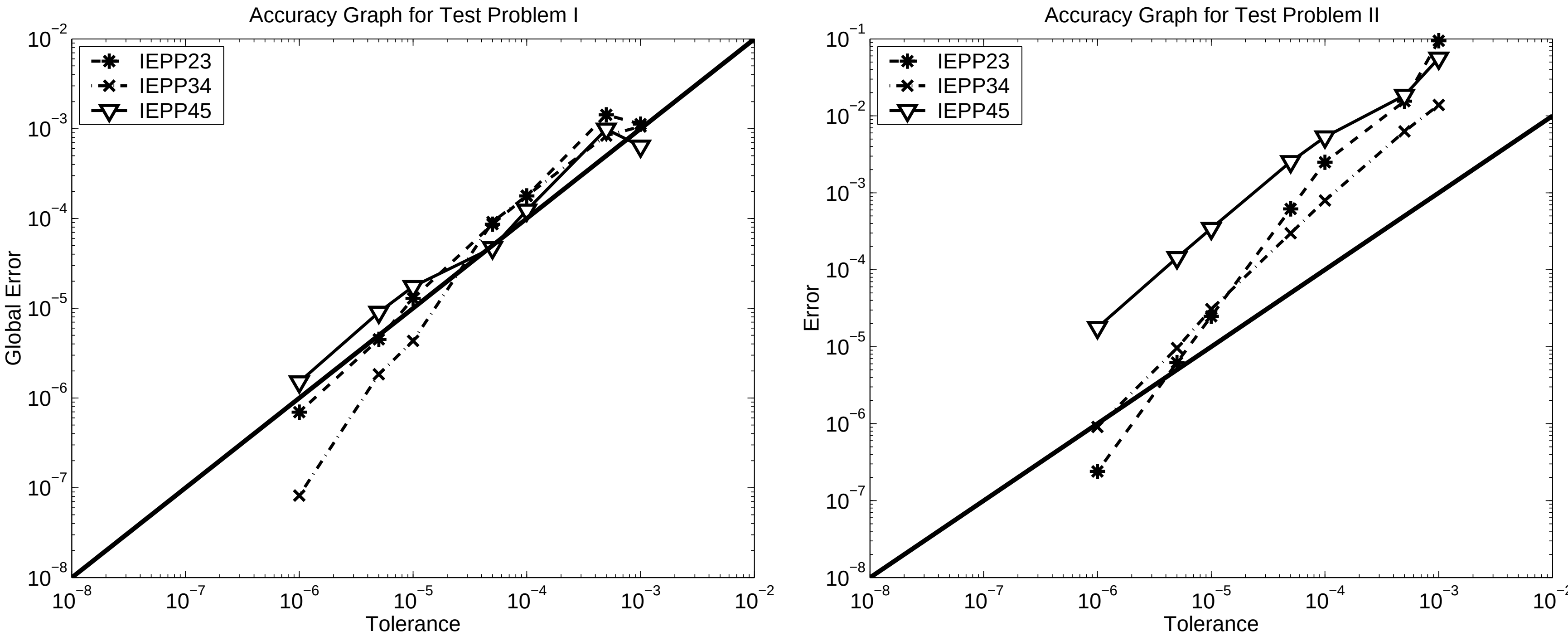

Figure 6. Exact errors of the embedded peer schemes with built-in our error estimation.

Efficient Global Error Control

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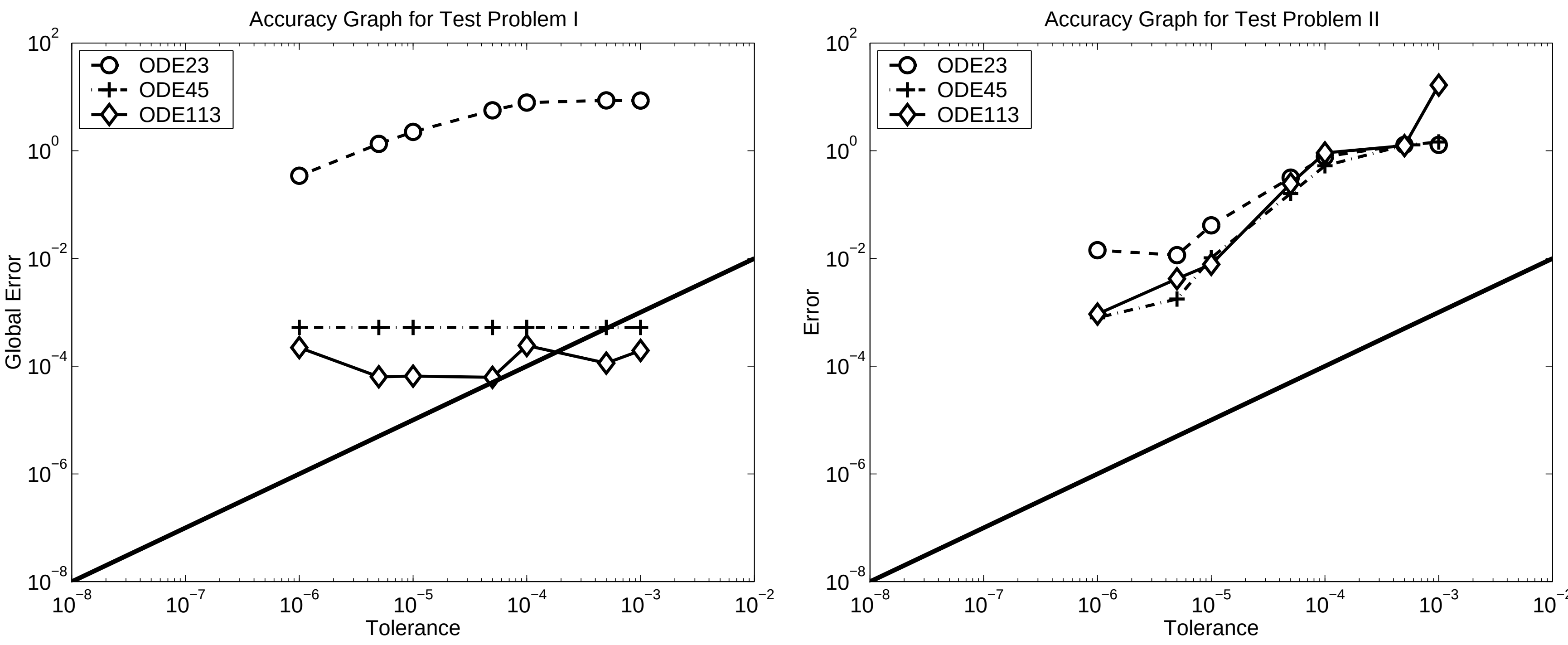

Figure 7. Exact errors of all explicit MatLab solvers with relative error control set by "RelTol"="AbsTol".

Efficient Global Error Control

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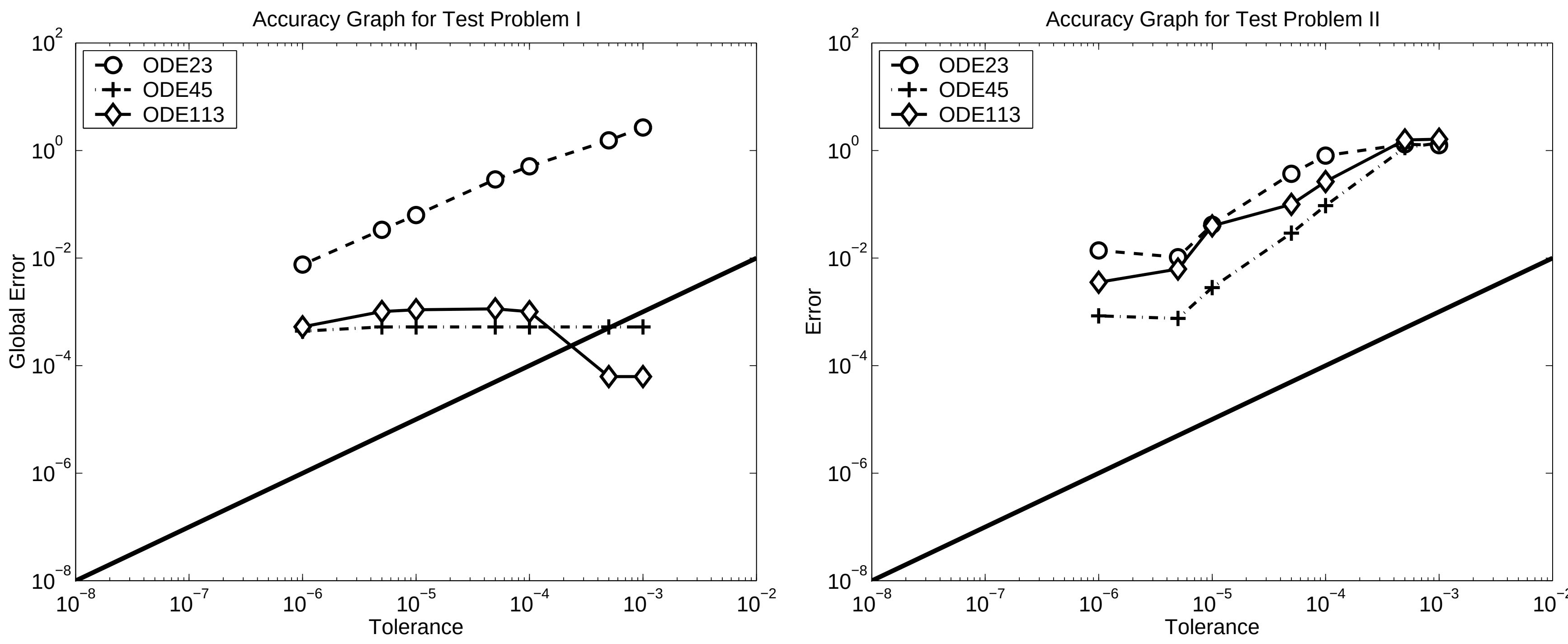

Figure 8. Exact errors of all explicit MatLab solvers without relative error control set by "RelTol":$= 1.0E - 10$.

Conclusion

IN THIS PAPER:

- We have discussed **the importance and power of double quasi-consistency** for efficient integration of differential equations. We have shown here that **the global error control** can be done for one computation of the integration interval.

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- We have discussed **the importance and power of double quasi-consistency** for efficient integration of differential equations. We have shown here that **the global error control** can be done for one computation of the integration interval.
- At first, we have proved **the existence** of doubly quasi-consistent schemes in the class of fixed-stepsize explicit parallel peer methods.

Conclusion

IN THIS PAPER (cont.):

- Then, we have explained how to accommodate the double quasi-consistency to **variable-stepsize explicit parallel peer methods of interpolation type**.

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IN THIS PAPER (cont.):

- Then, we have explained how to accommodate the double quasi-consistency to **variable-stepsize explicit parallel peer methods of interpolation type**.
- Our experiments have confirmed that **the usual local error control** can be very powerful when applied in **doubly quasi-consistent numerical schemes**.

Related References

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