Advances in Numerical Solution of Kinetics Reactions

MAMS - Technical Report

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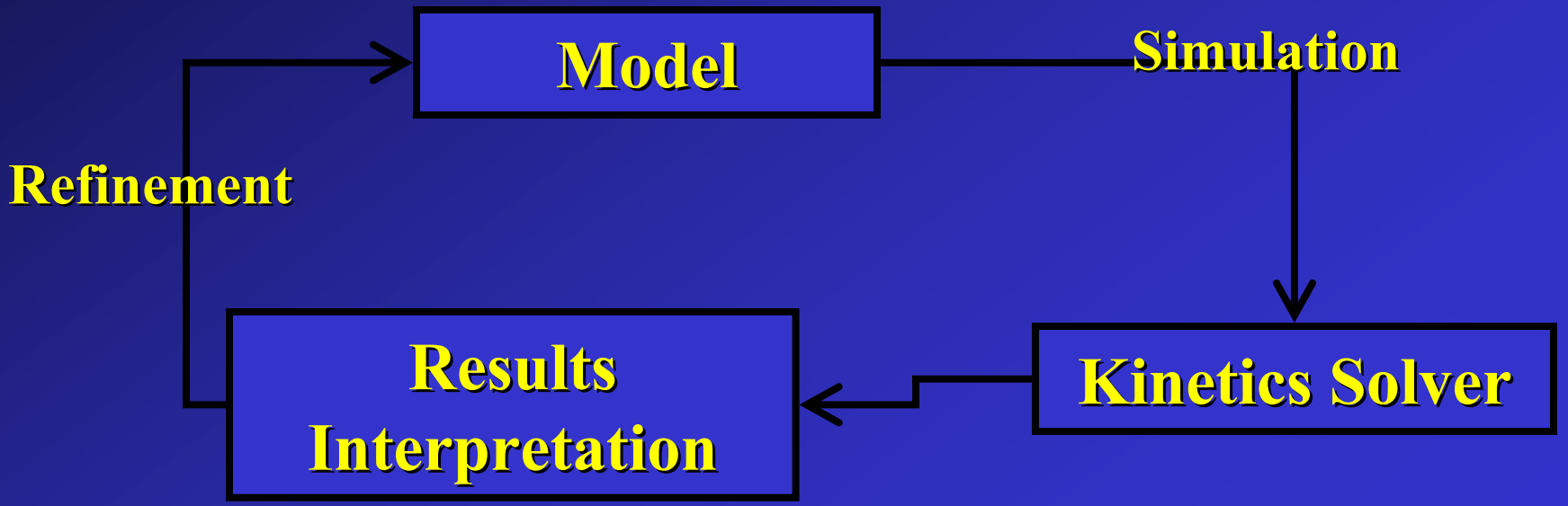
Agenda

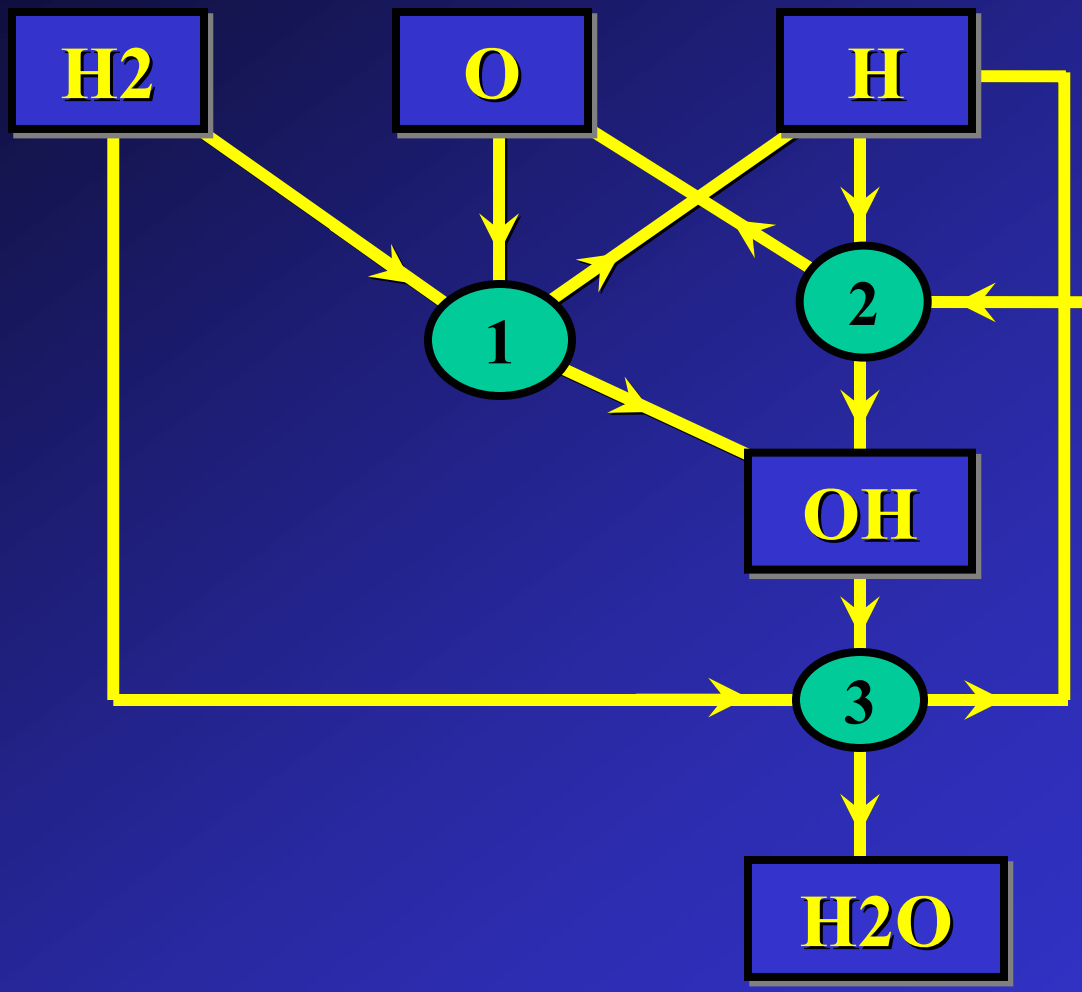
- Introduction
- Numerical Solution
- Graphics of the Solution
- Conclusions

Introduction

- Biochemical signaling networks
- Model Representation



Basic Model

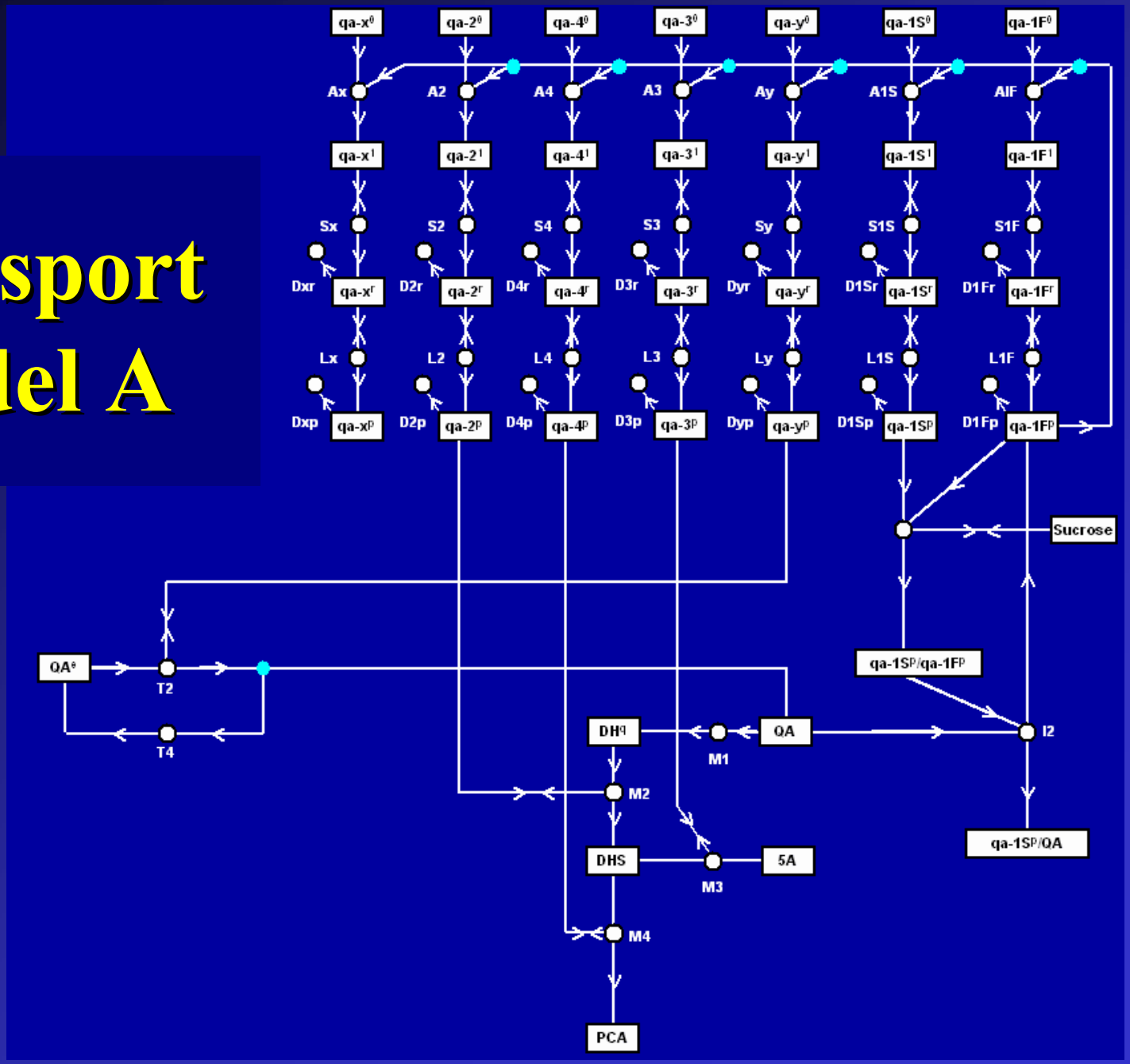


H2 + O ⇌ H + OH

H + O2 ⇌ O + OH

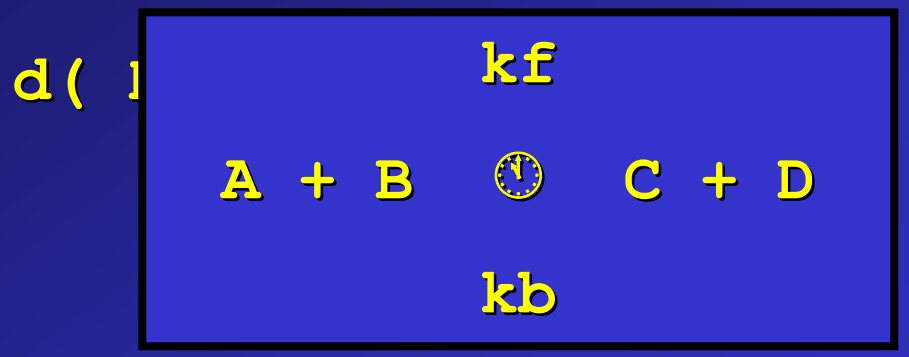
H2 + OH ⇌ H + H2O

Transport Model A

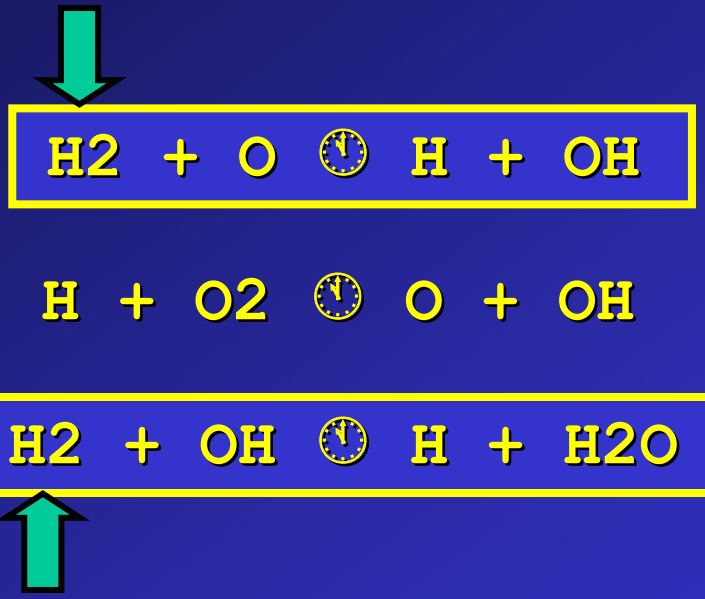


Reactions → Equations

- **Rate constants**
  - forward
  - backward



$$\frac{d[\,]}{} = k_f [O][OH] - k_b [OH] + k_{b_3} [H][H_2O]$$



Reactions → Equations

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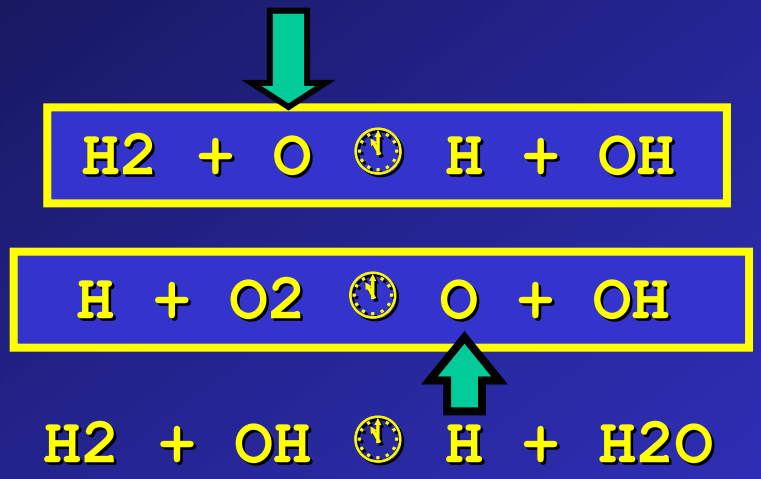


$$\frac{d[O]}{dt} = -kf_1[H2][O] + kb_1[H][OH] + kf_2[H][O2] - kb_2[O][OH]$$

Kinetics Solver

- Simulate kinetics reactions like:

$$H2 + O \rightleftharpoons H + OH$$

$$H + O2 \rightleftharpoons O + OH$$

$$H2 + OH \rightleftharpoons H + H2O$$

- Initial Time → Final Time
- Initial Concentrations and rate constants
- Numerical Method selection

Numerical Solution

Numerical Methods

- **Euler Method**

  $y_{n+1} = y_n + h\, f(t_n, y_n)$

- **Modified Euler**

  $k_0 = h\, f(t_n, y_n)$

  $k_1 = h\, f(t_n, y_n + k_0)$

  $y_{n+1} = y_n + \frac{1}{2}(k_0 + k_1)$

Numerical Methods ...

- **Fourth order Runge-Kutta**

$$k_1 = h\, f(t_n, y_n)$$

$$k_2 = h\, f(t_n + \tfrac{1}{2} h, y_n + \tfrac{1}{2} k_1)$$

$$k_3 = h\, f(t_n + \tfrac{1}{2} h, y_n + \tfrac{1}{2} k_2)$$

$$k_4 = h\, f(t_n + h, y_n + k_3)$$

$$y_{n+1} = y_n + (1/6)\,(k_1 + 2\,k_2 + 2\,k_3 + k_4)$$

Numerical Methods ...

- **Adaptive Runge-Kutta Fehlberg**

$k_1 = h\, f(t_n, y_n)$

$k_2 = h\, f(t_n + \frac{1}{4} h, y_n + \frac{1}{4} k_1)$

$k_3 = h\, f(t_n + c_1 h, y_n + c_2 k_1 + c_3 k_2)$

$k_4 = h\, f(t_n + c_4 h, y_n + c_5 k_1 + c_6 k_2 + c_7 k_3)$

$k_5 = h\, f(t_n + h, y_n + c_8 k_1 + c_9 k_2 + c_{10} k_3 + c_{11} k_4)$

$k_6 = h\, f(t_n + \frac{1}{2} h, y_n + c_{12} k_1 + 2 k_2 + c_{13} k_3 + c_{12} k_4 + c_{13} k_5)$

4th $y_{n+1} = y_n + c_{14} k_1 + c_{15} k_2 + c_{16} k_3 + c_{17} k_4$

5th $y_{n+1} = y_n + c_{18} k_1 + c_{19} k_3 + c_{20} k_5 + c_{21} k_6$

Numerical Methods ...

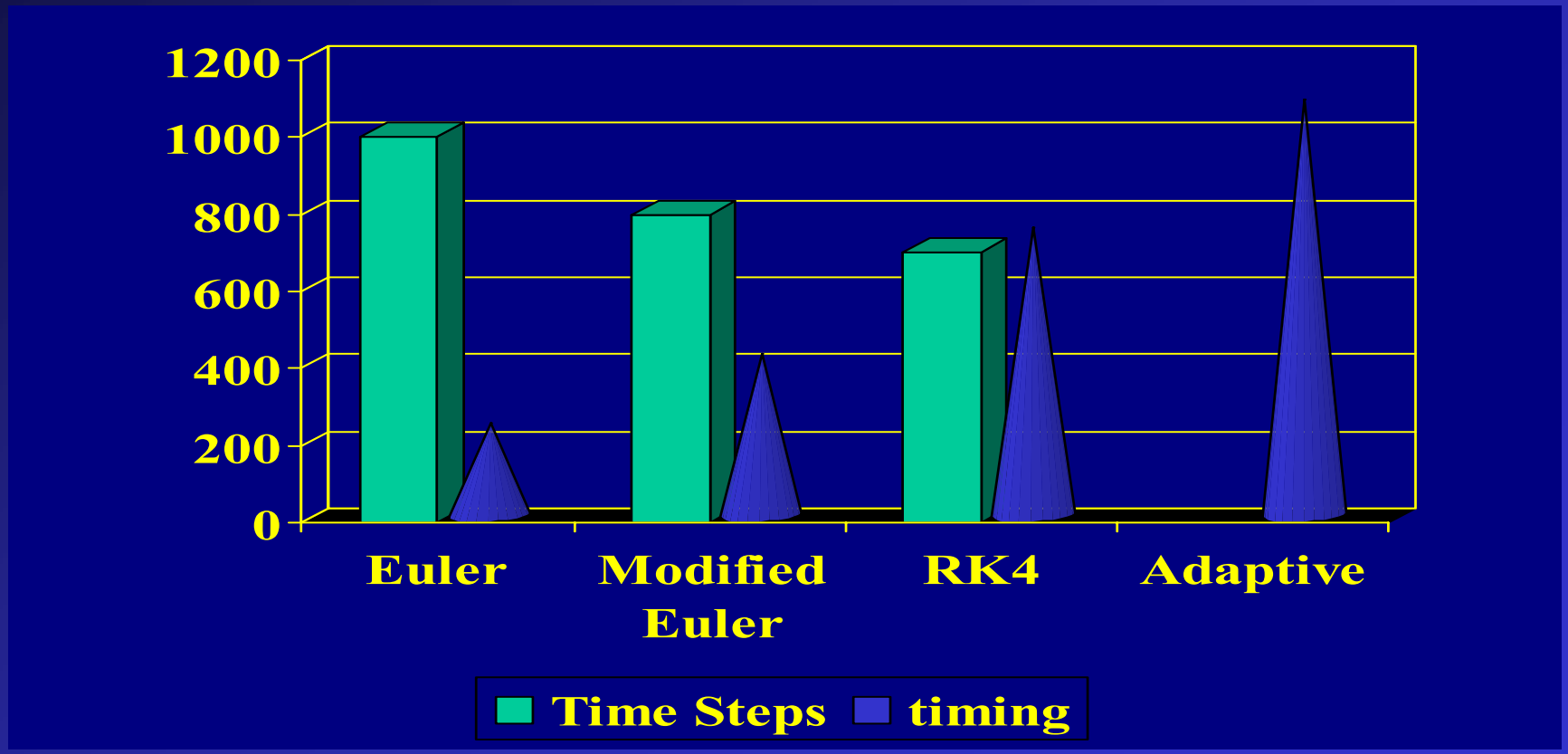
- **Backward Difference Formula (Implicit)**

  $y_{n+1} = (4/3)\, y_n - (1/3)\, y_{n-1} + (2/3)\, y'_{n+1}$

  - **Jacobian evaluation**
  - **System of Equations: $O(m^3) + O(m^2)$**

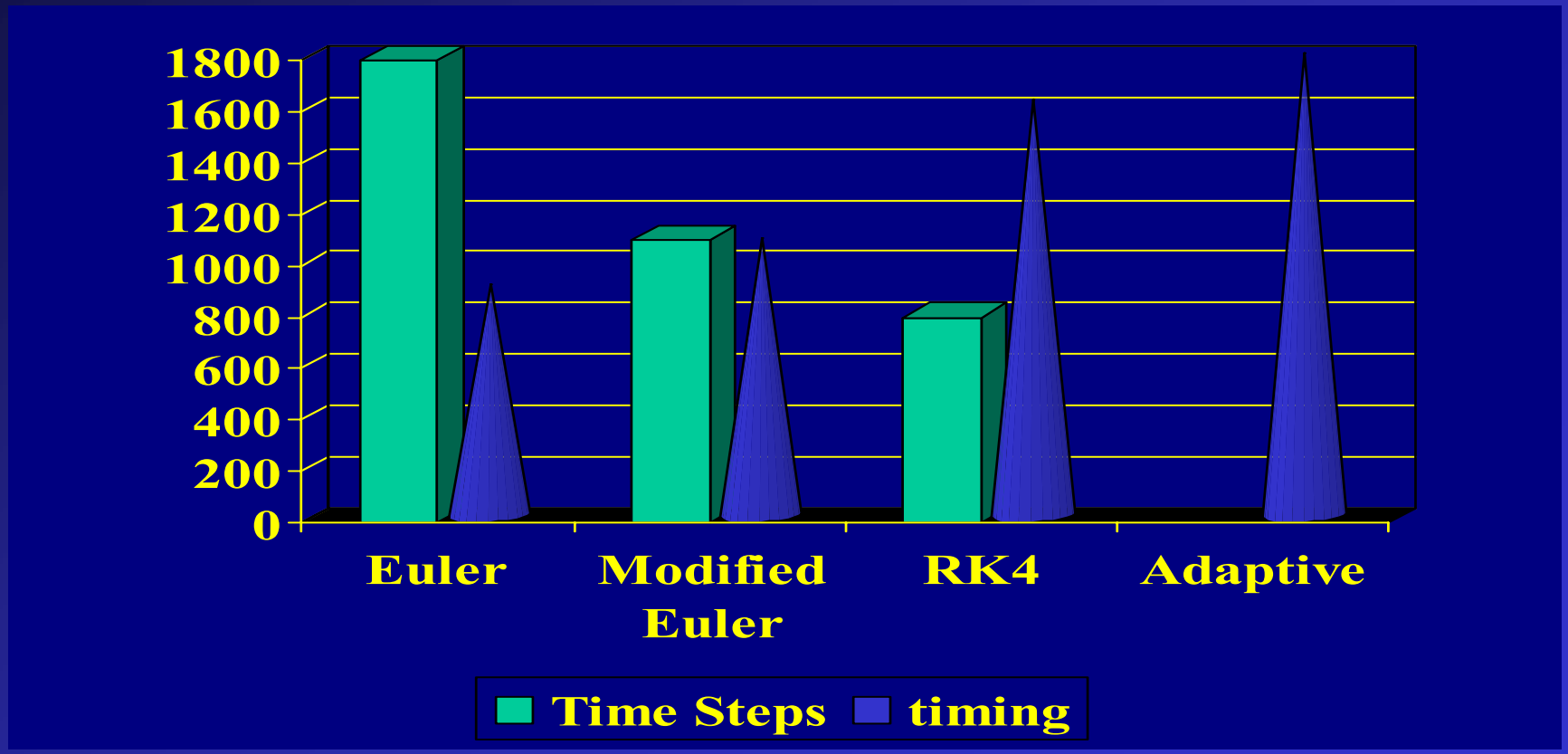
Performance

- With data set QA-Tr.B



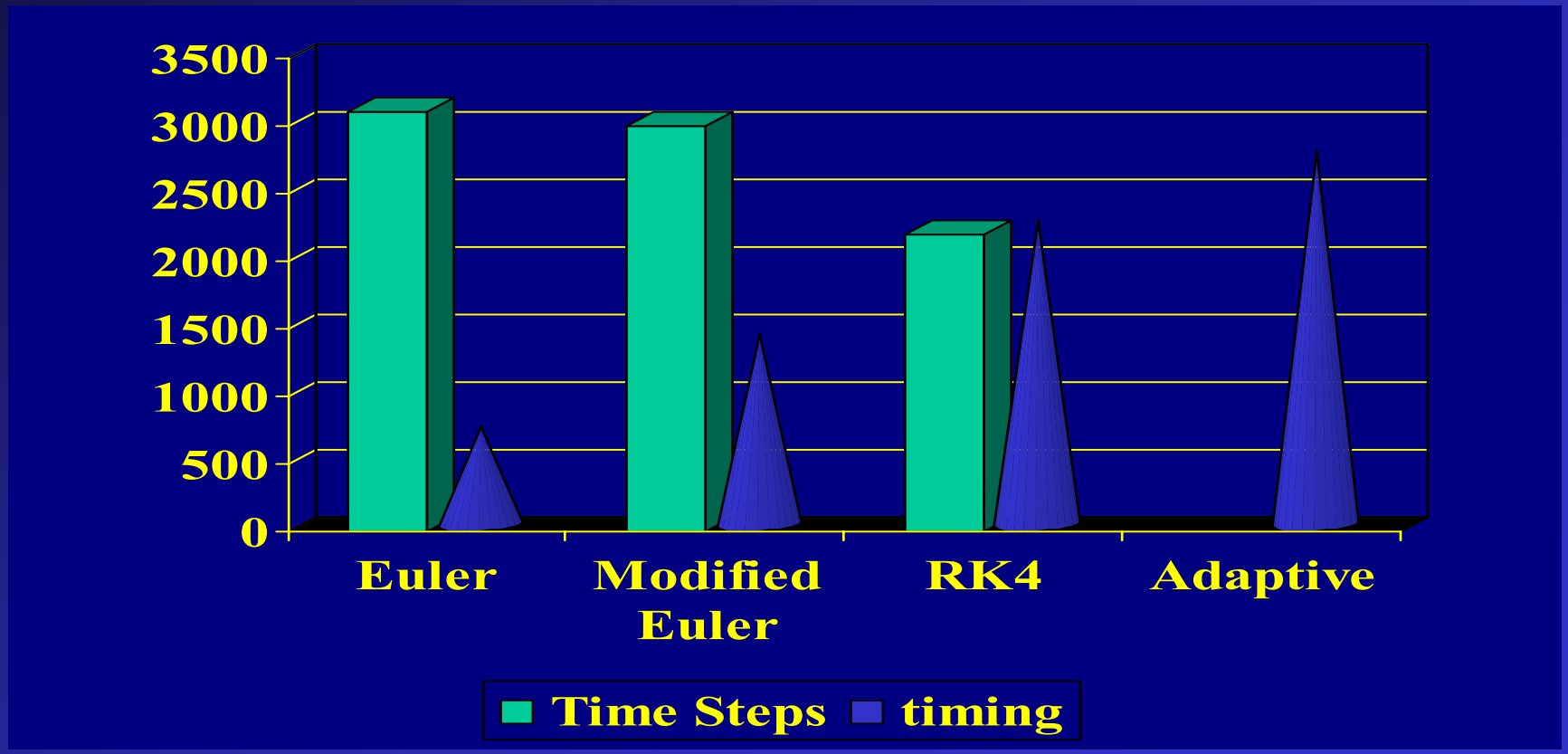
Performance

- With data set QA-A



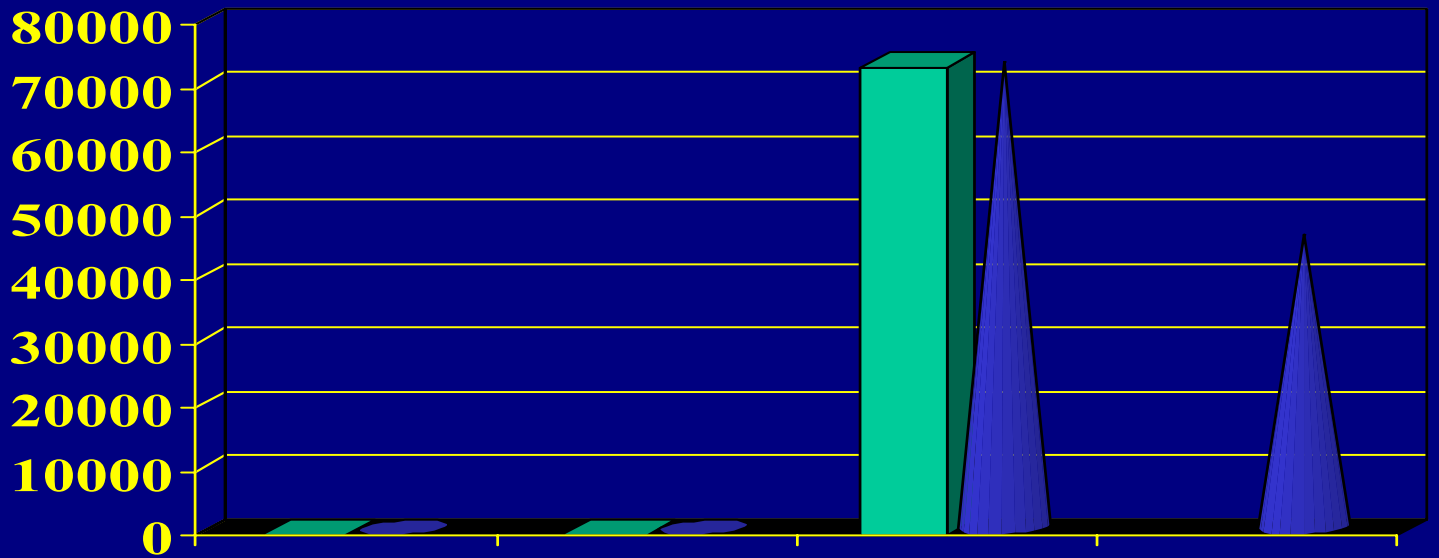
Performance

- With data set QA-Tr.-A



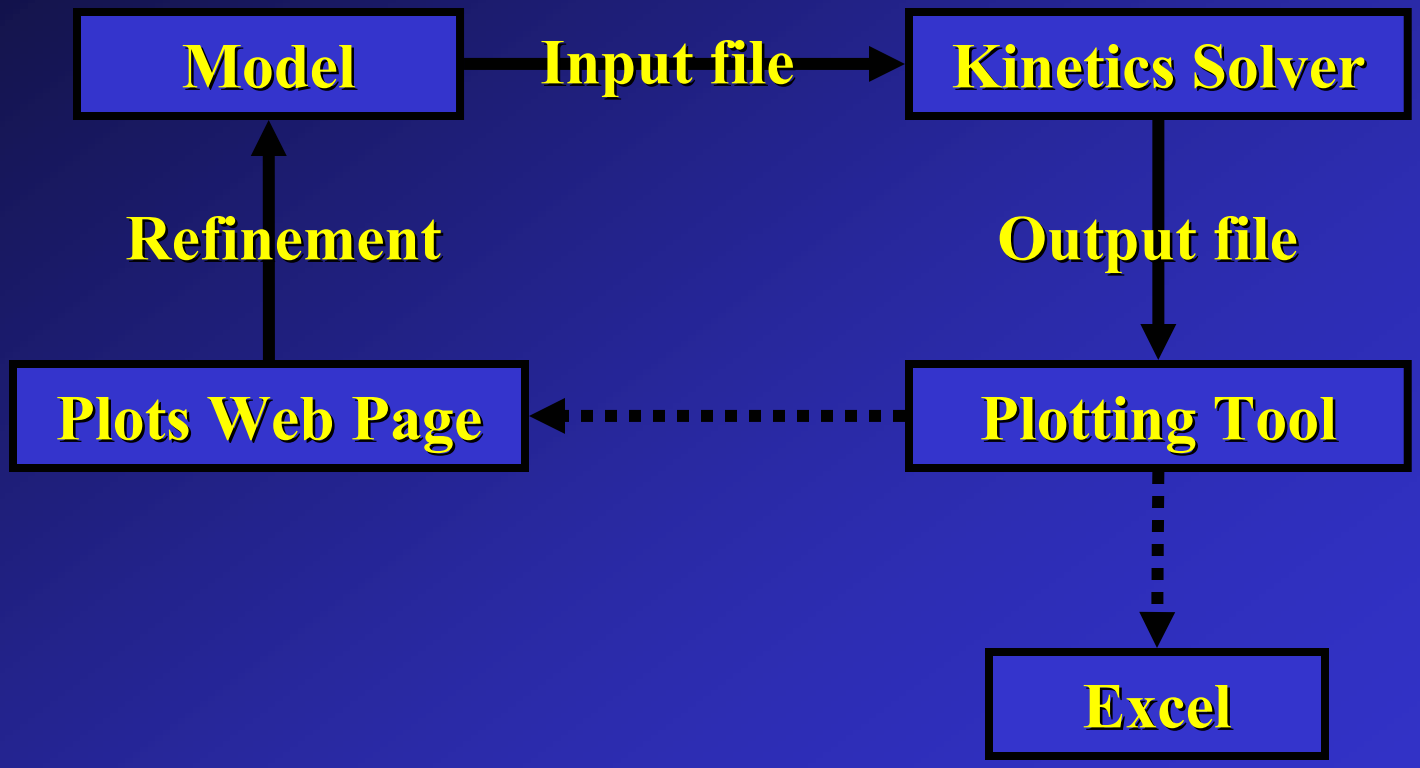
Performance

- With data set LAC-PTS

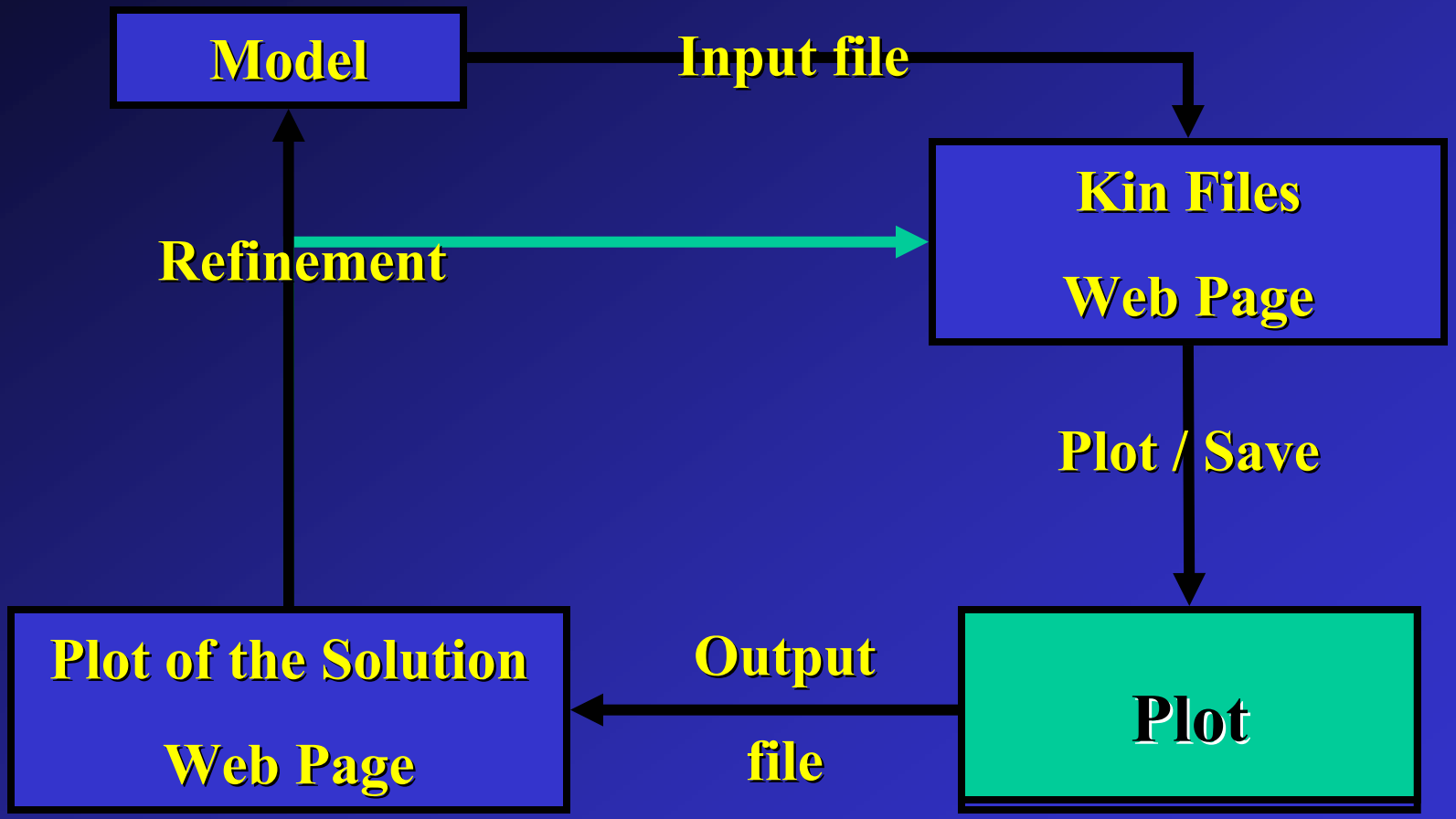


Graphics of the Solution

Using the Kinetics Solver



Using the Kinetics Solver ...



Conclusions

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- Numerical methods :
  - performance vs. accuracy
  - data set parameters

  - Stiff solver inadequate
- Plotting by Web Page
- “Computing Life”

Questions and Comments!