Building Exponential Integrators to Solve Large Stiff Systems of Differential Equations

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2 hrs

1.5 hrs

Outline:

- *Motivation*
- *Numerical methods for stiff problems*
- *Construction and performance of exponential integrators*

What is Stiffness? And Where Do We Encounter It?

- There are many definitions of stiffness, e.g

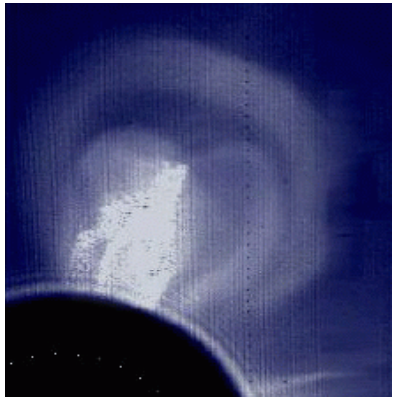
  Lambert'91: A problem is stiff on a particular interval if a numerical method is forced to use an excessively small step size in relation to the smoothness of the solution.

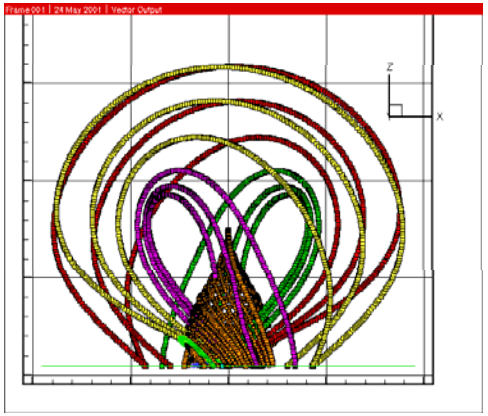
- Stiff problems are encountered in many fields, e.g.

Plasma physics

Combustion

Fluid Mechanics





General Nonlinear Problem:

$$\frac{dy}{dx} = f(y) \qquad y \in \mathbb{R}^N$$
$$y(x_0) = y_0 \qquad N >> 1$$

- stiff, stiffness can come from either linear OR nonlinear part $f(y) = Ly + N(y)$

$$\Delta t_{Stability} << \Delta t_{Accuracy}$$

- no efficient preconditioner is available for implicit methods

Elementary Example:

1D Heat Equation $\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2}$

Discretized in space

$$\frac{dU}{dt} = AU \qquad A = \frac{\nu}{\Delta x^2}\begin{bmatrix} -2 & 1 & \dots & 0 \\ 1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 0 & \dots & 1 & -2 \end{bmatrix}$$

Explicit scheme

$$\boxed{\begin{aligned} U^{n+1} &= U^n + A\Delta t U^n \\ U^{n+1} &= (I + A\Delta t)U^n \end{aligned}}$$

Implicit scheme

$$\boxed{\begin{aligned} U^{n+1} &= U^n + A\Delta t U^{n+1} \\ U^{n+1} &= (I - A\Delta t)^{-1}U^n \end{aligned}}$$

But there is also exact solution!

$$U^{n+1} = e^{A\Delta t}U^n$$

Numerical Difficulties with Stiffness:

Eigenvalues of A place stability restriction on the time step for the explicit scheme

$$\mu_k = -\frac{4\nu}{(\Delta x)^2}\left(\sin\left(\frac{\pi k}{2(N+1)}\right)\right)^2$$

Explicit scheme

$$U^{n+1} = (I + A\Delta t)U^n$$

Stability requirement

$$|1 + \mu_k \Delta t| < 1$$

Implicit scheme VS. Exponential integrator

$$U^{n+1} = (I - A\Delta t)^{-1}U^n$$

$$U^{n+1} = e^{A\Delta t}U^n$$

Both A-stable but…

Implicit vs. Exponential schemes:

Since A is large we need to approximate

$$(I - A\Delta t)^{-1}b = (I + (A\Delta t) + (A\Delta t)^2 + (A\Delta t)^3 + \ldots)b$$

or

$$e^{A\Delta t}b = \left(I + \frac{(A\Delta t)}{1!} + \frac{(A\Delta t)^2}{2!} + \frac{(A\Delta t)^3}{3!} + \ldots\right)b$$

Approximation method of choice for large nonsymmetric matrices is Krylov subspace projection

$$S_k = span\{b, Ab, \ldots, A^{k-1}b\}$$

(i.e. to invert the matrix we can use GMRES or FOM)

Convergence of Krylov iteration to estimate f(A)b depends on ||b||, eigenvalues of A *and function f(x)!*

Test problem – 2D Brusselator:

$$\frac{du_i}{dt} = 1 + u_i^2 v_i - 4u_i + \alpha \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2}$$

$$\frac{dv_i}{dt} = 3u_i - u_i^2 v_i + \alpha \frac{v_{i-1} - 2v_i + v_{i+1}}{(\Delta x)^2}, \quad i = 1, ..., N$$

Jacobian matrix:

$$J = \begin{bmatrix} diag(2u_i v_i - 4) & diag(u_i^2) \\ diag(3 - u_i v_i) & diag(-u_i^2) \end{bmatrix} + \frac{\alpha}{(\Delta x)^2} \begin{bmatrix} L & 0 \\ 0 & L \end{bmatrix}$$

$$L = \begin{bmatrix} -2 & 1 & \dots & 0 \\ 1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 0 & \dots & 1 & -2 \end{bmatrix}$$

Krylov iteration convergence comparison:

Tolerance = 1E-5

Problem size, 2N	GMRES $(I - A\Delta t)^{-1}b$	FOM $(I - A\Delta t)^{-1}b$	$e^{A\Delta t}b$	$\psi_{21}(A\Delta t)b$	$\psi_{22}(A\Delta t)b$
200	92	85	35	27	19
400	187	174	70	55	38
800	382	359	140	112	78

Similar result also holds for Jacobian calculated at different times and for other examples.

Building Exponential Integrators:

$$\frac{dy}{dx} = f(y) = Ly + N(y)$$

$$y(x_0 + h) = e^{hL} y_0 + \int_{x_0}^{x_0+h} e^{(x_0+h-s)L} N(y(s))ds$$

OR

$$\frac{dy}{dx} = f(y) = f(y_0) + \frac{Df}{Dy}(y_0)(y - y_0) + R(y)$$

$$y(x_0 + h) = y_0 + \frac{e^{hA_0} - I}{hA_0} hf(y_0) + \int_{x_0}^{x_0+h} e^{(x_0+h-s)A_0} R(y(s))ds$$

Building Exponential Integrators:

$$y(x_0+h) = y_0 + \frac{e^{hA_0} - I}{hA_0} h f(y_0) + \int_{x_0}^{x_0+h} e^{(x_0+h-s)A_0} R(y(s)) ds$$

To construct an exponential method approximate $R(y(s))$ with a polynomial.

This results in a expression for an approximate solution which involves functions

$$\phi_k(z) = \int_0^1 e^{(1-s)z} \frac{s^{k-1}}{(k-1)!} ds$$

or their linear combinations, e.g.

$$\psi_{\gamma k}(z) = \int_0^1 e^{(1-s)z} \binom{\gamma s}{k} ds$$

Examples of EIs – Tokman:

$$
\begin{aligned}
R(y) &= f(y) - f(y_n) - A_n(y - y_n) \\
k_1 &= y_n + a_{11}\psi_1(hA_n/3)hf(y_n) \\
k_2 &= y_n + a_{21}\psi_1(2hA_n/3)hf(y_n) + a_{22}\psi_2(2hA_n/3)hR(k_1) \\
y_{n+1} &= y_n + b_1\psi_1(hA_n)hf(y_n) + b_2\psi_2(hA_n)hR(k_1) \\
&+ b_3\psi_3(hA_n)h(-2R(k_1) + R(k_2))
\end{aligned}
$$

$$
\begin{aligned}
\psi_1(z) &= \phi_1(z) \\
\psi_2(z) &= 3\phi_2(z) \\
\psi_3(z) &= 3/2(-\phi_3(z) + 6\phi_2(z))
\end{aligned}
$$

Fourth-order scheme EPIRK4 – 3 Krylov projections

Methods Performance Comparison for Brusselator Example:

Method	Time	Error	Time	Error	Time	Error
AM2	7.81	0.014	9.72	0.013	12.8	0.013
AM2IN	1.93	0.012	2.62	0.013	3.49	0.013
EPI2	0.44	0.011	0.56	0.008	0.67	0.085
EPI3	0.56	0.010	0.67	0.0017	0.87	0.001
EPIRK3	0.59	0.011	0.71	0.0023	0.99	0.0008

More Tests:

2D Brusselator

$$\frac{\partial u}{\partial t} = 1 + uv^2 - 4u + \alpha\nabla^2 u$$
$$\frac{\partial v}{\partial t} = 3u - u^2 v + \alpha\nabla^2 v$$

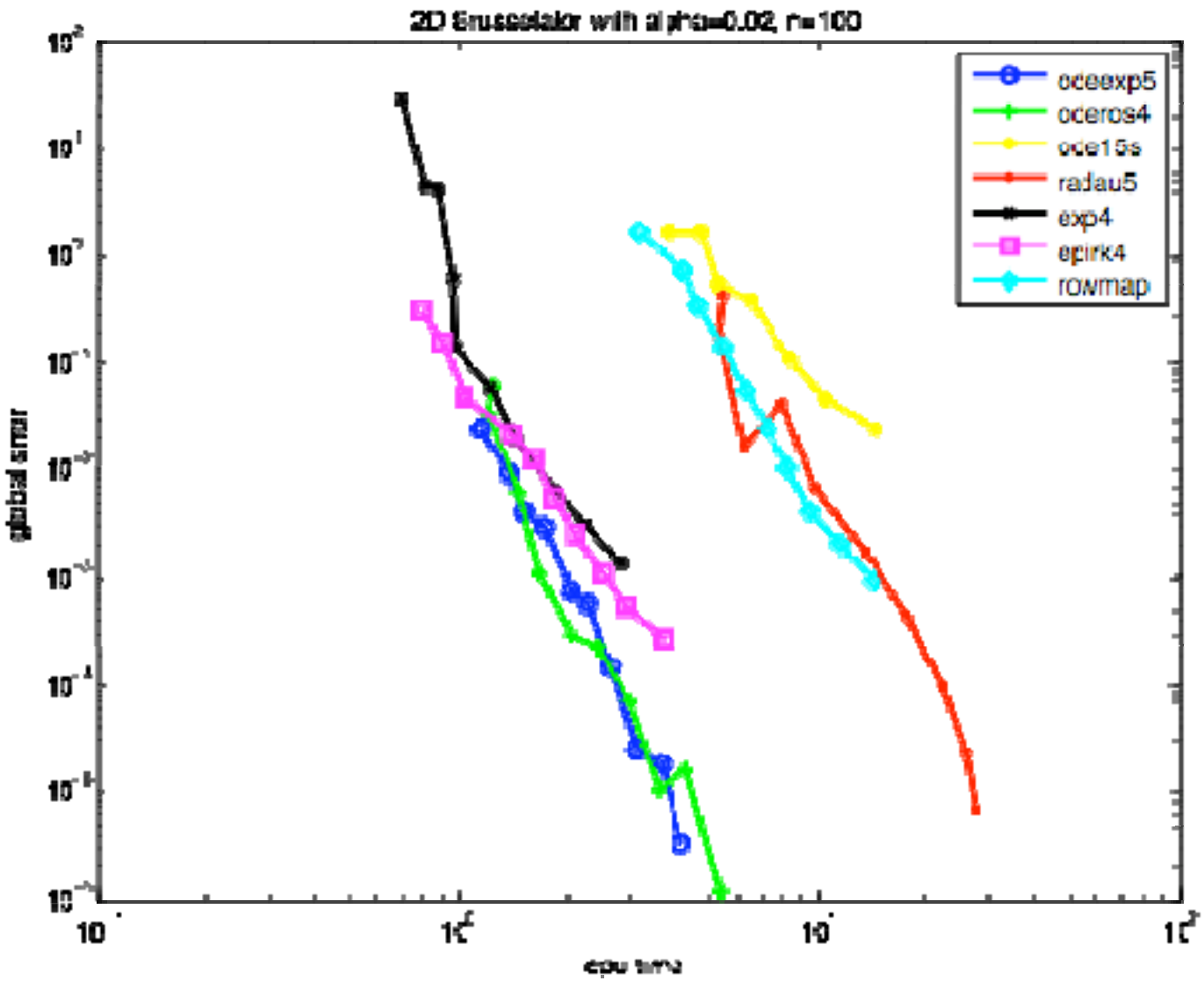
2D Gray-Scott Equation

$$\frac{\partial u}{\partial t} = -uv^2 + 0.04(1-u) + 0.2\nabla^2 u$$
$$\frac{\partial v}{\partial t} = uv^2 = 0.1v + 0.1\nabla^2 v$$

2D Allen-Cahn Equation

$$\frac{\partial u}{\partial t} = u - u^3 + 0.1\nabla^2 u$$

2D Brusselator:



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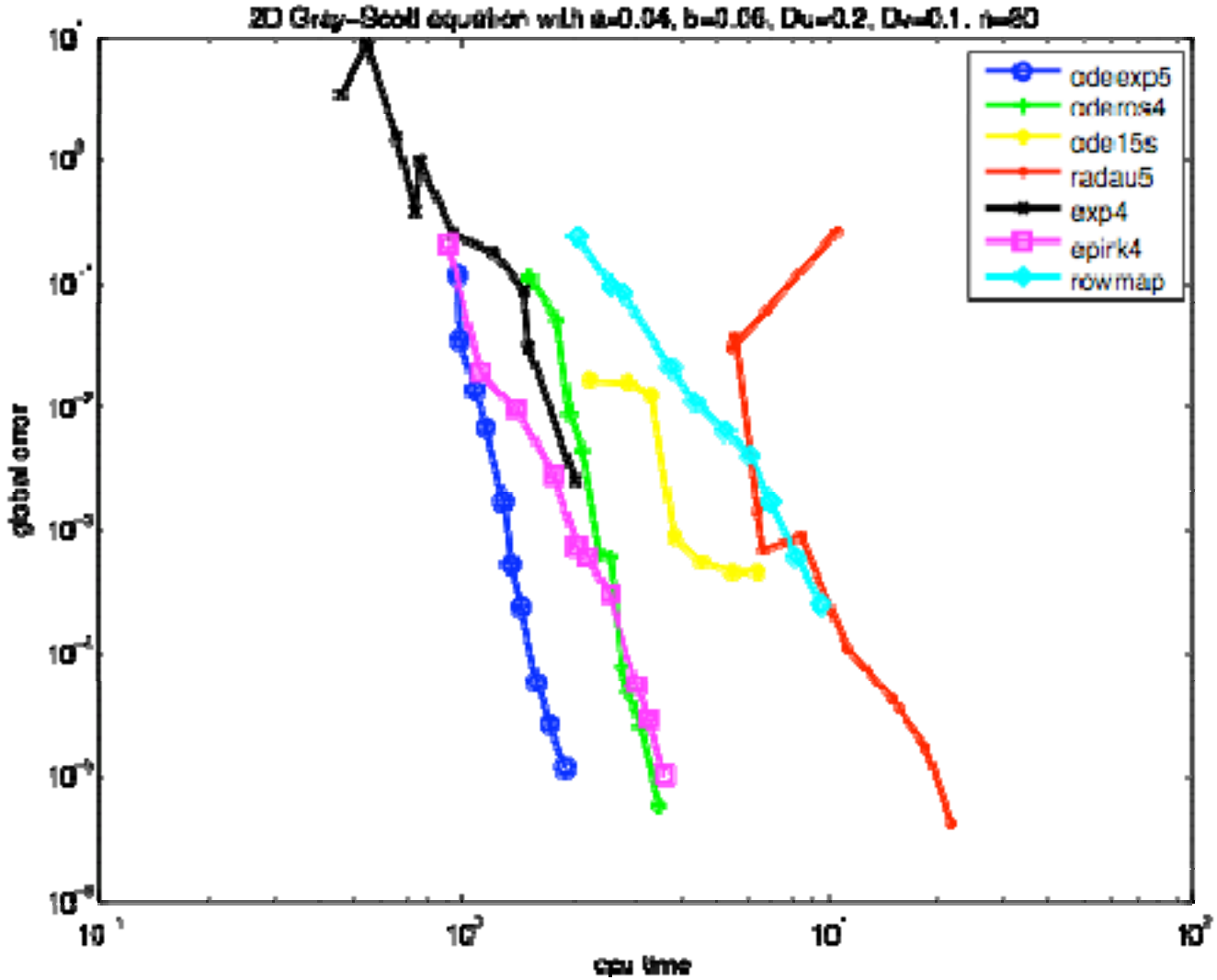

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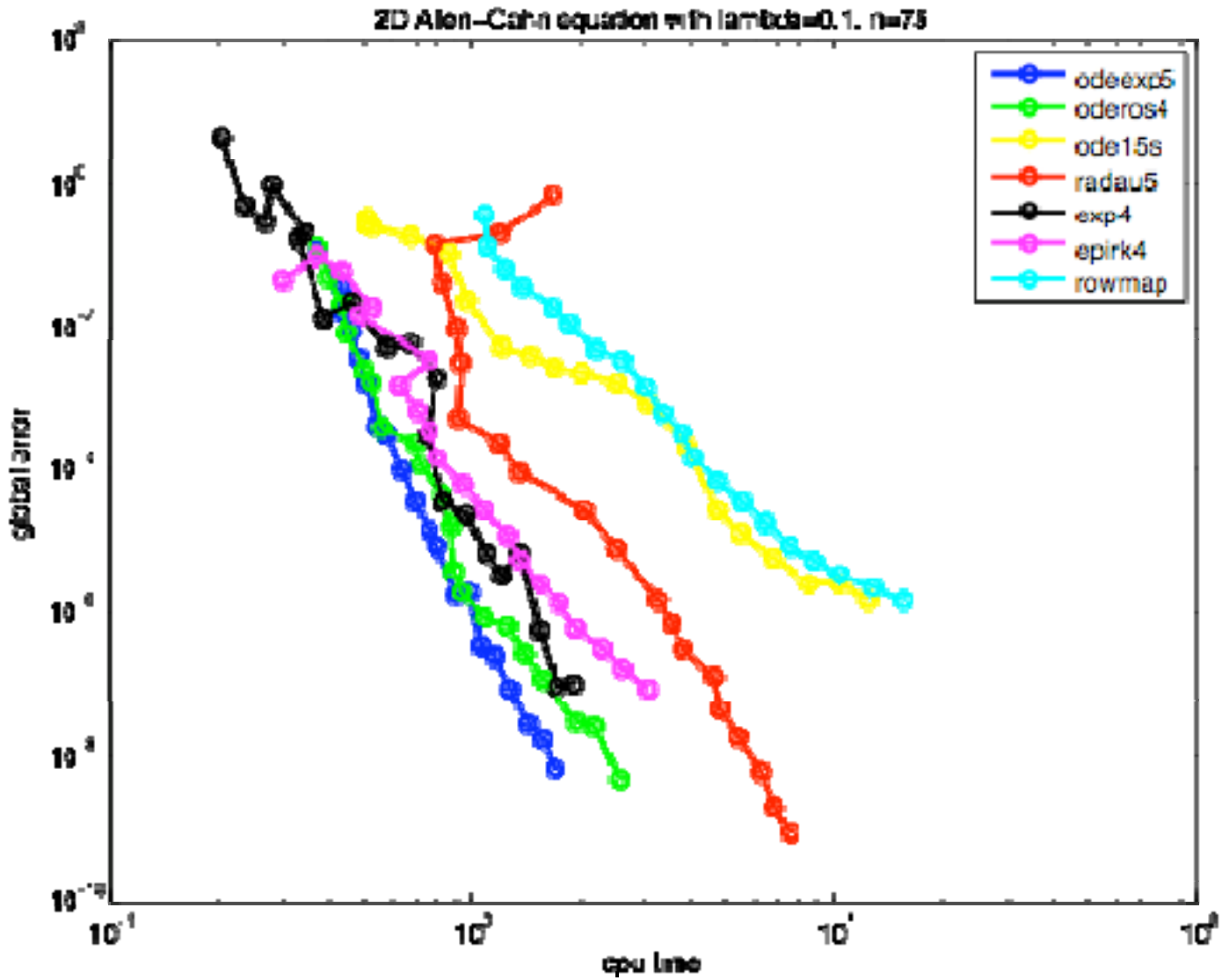
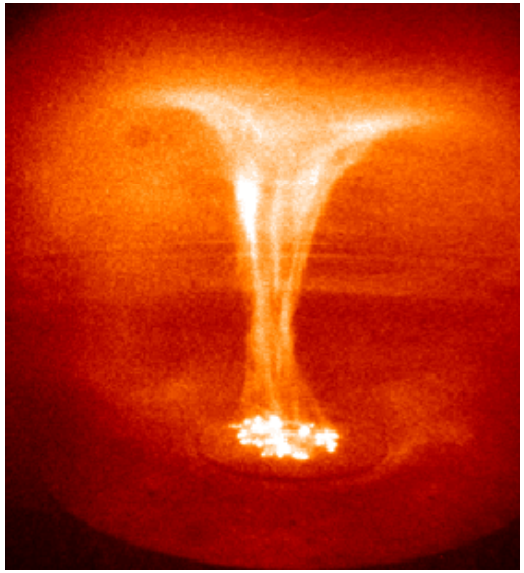
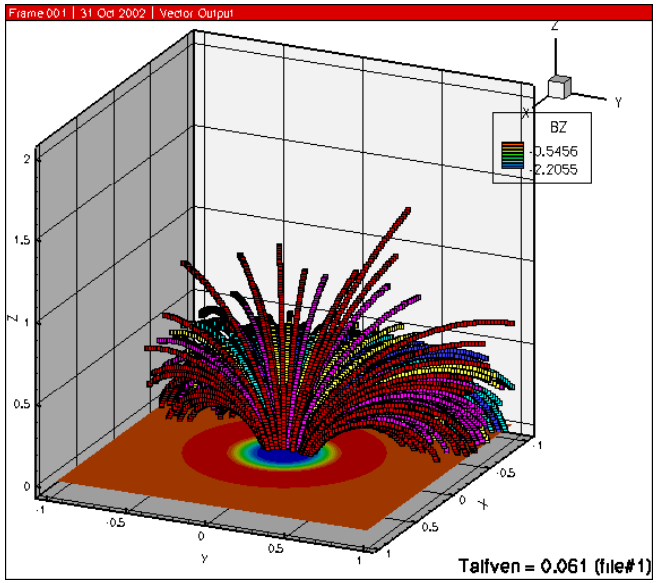


Conclusions and Future Work:

- Thorough comparisons of EIs and standard integrators performance on both *test problems and real applications*
- Construction and analysis of new exponential methods
- Development of publically available *serial and parallel* implementation of EIs





History and Related Work:

Linear or Small Systems:

Certaine '60, Pope '63, Lawson '67, Norsett '69, Nautts & Wyatt '83, Park & Light '86, Saad '96

Semilinear Systems:

e.g. Gallopoulos & Saad '92, Lawson et al. 94, Beylkin et al ' 98, Cox & Matthews '02, Kassam & Trefethen '04, Hochbruck & Ostermann'05, Ostermann, Thalhammer & Wright '06,

General Nonlinear Systems:

Edwards et al. '94, Hochbruck & Lubich '98, Tokman'06, Hochbruck & Ostermann'06

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Lambert'91: A problem is stiff on a particular interval if a numerical method is forced to use an excessively small step size in relation to the smoothness of the solution.

Gear'71: Model problem

$$y'(t) = A(y - F(t)) + F'(t)$$

Eigenvalues of the Jacobian define stiffness ratio

$$S = \frac{\max |Re\lambda_i|}{\min |Re\lambda_i|}$$

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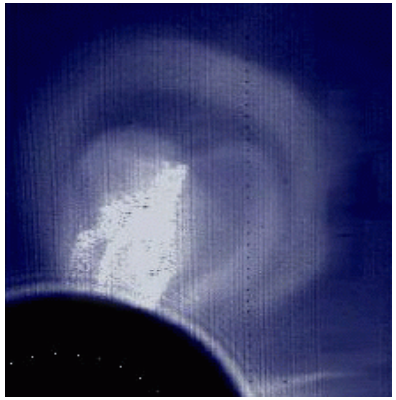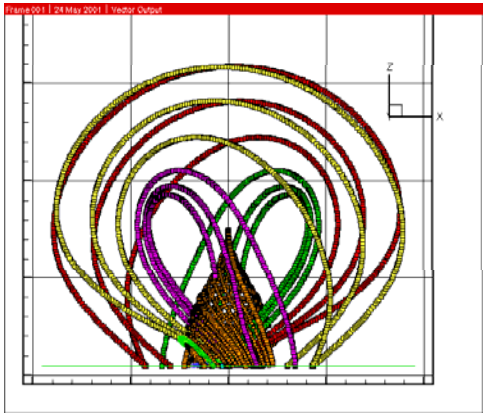
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