NASA GSRP Final Report (6/27/04)

(1) Name and Grant Number:

Alex Kanevsky, NGT-1-01024

(2) Dates of Fellowship and Degrees Received:

GSRP: 7/01/2001 – 6/30/2004.
Degree: M.Sc. in Applied Mathematics, 5/2001.

(3) Title:

Overcoming Geometry-Induced Stiffness with IMplicit-EXplicit (IMEX) Runge-Kutta Algorithms on Unstructured Grids with Applications to CEM, CFD, and CAA.

(4) NASA Research Advisor:

Dr. Mark H. Carpenter

(5) Conference Participation:

International Conference on Spectral and High Order Methods (ICOSAHOM), Brown University, Providence, RI, June 21-25, 2004.

AFOSR Workshop on Advances and Challenges in Time-Integration of PDE's, Brown University, Providence, RI, August 18-20, 2003.

NASA GSRP Orientation and Workshop, Hampton, VA, July 2003.

Second MIT Conference on Computational Fluid and Solid Mechanics, Cambridge, MA, June 17-20, 2003.

ICASE's 30th Anniversary Conference, Hampton, VA, August 2002.

NASA GSRP Orientation and Workshop, Hampton, VA, July 24-26, 2002.

SIAM 50th Anniversary and 2002 Annual Meeting, Philadelphia, PA, July 8-12, 2002.

International Conference on Scientific Computing, Partial Differential Equations and Image Processing, On the Occasion of Stanley Osher's 60^{th} birthday, UCLA, April 5-7, 2002.

Ninth International Conference on Hyperbolic Problems: Theory, Numerics, Applications. California Institute of Technology, Pasadena, CA, March 25-29, 2002.

NASA GSRP Orientation and Workshop, Hampton, VA, July 25-27, 2001.

(6) Seminars or Lectures:

Seminar given at NASA GSRP Orientation and Workshop, Hampton, VA, July 2003.

(7) Meetings Attended By Invitation:

N/A

(8) Teaching Experience:

(a) Instructor, Introduction to Computing Sciences (AM 16), Brown University, Spring 2004.

(b) Teaching Assistant, Methods in Applied Math I (AM 33), Brown University, Fall 2002.

(9) Summary of Research: See Attached Page.

(10) Publications and Papers:

Chauviere, C., Hesthaven, J.S., Kanevsky, A., and Warburton, T., *High-order localized time integration for grid-induced stiffness*, Proceedings of the Second MIT conference on Computational Fluid and Solid Mechanics (June 2003).

(11) Patents:

N/A

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(13) Appraisal of the GSRP:

The GSRP program has been incredibly valuable for my development as a scientist/researcher. I would like to thank all those individuals at NASA from the bottom of my heart who gave me such a wonderful opportunity. The most valuable aspect of the program was the mentoring I received from Dr. Mark H. Carpenter. Mark is a scientist of the highest caliber with incredible clarity, vision and creativity. He is also a very nice man. He really taught me a lot during all the times I came down during the summers and winters. I learned about the smaller and bigger pictures, including how to break down and analyze problems mathematically as well as what types of practical uses and applications IMEX methods have in science and engineering. I would like to thank him for all of these things.

I gained a lot from the annual GSRP conferences organized by Lloyd Evans and David Peterson. It was very beneficial to meet other GSRP participants and learn about their research. I also enjoyed the tours of NASA and all of the social activities. Thank you!

FACULTY ADVISER: J. S. Hesthaven DATE: 6/28/04

STUDENT: Alex Kanevsky DATE: 6/28/04

(9) Summary of Research:

My goal is to develop and implement efficient, accurate, and robust IMplicit-EXplicit Runge-Kutta (IMEX RK) methods [9] for overcoming geometry-induced stiffness with applications to computational electromagnetics (CEM), computational fluid dynamics (CFD) and computational aeroacoustics (CAA). IMEX algorithms solve the non-stiff portions of the domain using explicit methods, and isolate and solve the more expensive stiff portions using implicit methods.

Current algorithms in CEM can only simulate purely harmonic (up to 10GHz plane wave) EM scattering by fighter aircraft, which are assumed to be pure metallic shells, and cannot handle the inclusion of coatings, penetration into and radiation out of the aircraft. Efficient IMEX RK methods could potentially increase current CEM capabilities by 1-2 orders of magnitude, allowing scientists and engineers to attack more challenging and realistic problems.

This year, I completed my third year of research under the guidance of Professors David Gottlieb and Jan S. Hesthaven of Brown University and Dr. Mark H. Carpenter of NASA Langley Research Center. During the past 3 years, I implemented and tested explicit, implicit, and IMEX time-integration algorithms for solving linear as well as nonlinear equations in one and two dimensions on unstructured grids, such as burgers equation and the Euler equations, using Discontinuous Galerkin [3,4,5,8] spectral element spatial discretizations.

The Discontinuous Galerkin Spectral Element (DGSE) method builds upon the strengths and overcomes the weaknesses of the Discontinuous Galerkin Finite Element method [3, 4] and the classical spectral element method introduced by Patera [11, 12], and has a number of advantages over classical finite difference and finite volume methods. DGSE methods are especially well suited for IMEX algorithms, since they allow for clean and easy decoupling of the stiff from the nonstiff regions of the domain. Furthermore, they are highly parallelizable and accurate, provide for simple treatment of boundary conditions, handle complicated geometries well, and can easily handle adaptivity. Utilizing an unstructured grid [8] allows me to capture very fine details of complex domains, which is crucial for tackling real-world problems.

My research shows that when geometry-induced stiffness is significant (greater or equal to 2 orders of magnitude), IMEX algorithms [9] outperform traditional explicit time-stepping RK methods by about an order of magnitude or more in 1D for systems having smooth solutions. I also found that Krylov subspace iterative methods, such as GMRES and BiCGStab, in conjunction with good preconditioners are essential in order to achieve this kind of speedup. Some of the results from my research have been presented at the Second MIT conference on Computational Fluid and Solid Mechanics and are published in [2].

In 2D, IMEX methods outperform explicit methods even without preconditioning (when geometry-induced stiffness is greater than 1-2 orders of magnitude) for problems having smooth solutions. When shocks are present, the situation is not as clear since Newton's method often fails to converge and many steps must be repeated with smaller time-steps. Preconditioning gives IMEX methods an even greater computational advantage in two dimensions. ILU preconditioners worked very well in 1D, while Jacobi, Gauss-Seidel and block-Jacobi preconditioners were not as effective. I will need to further investigate effective 2D and 3D preconditioning techniques such as multigrid-based preconditioners [10].

I am currently developing and testing time advancement algorithms for solving systems of nonlinear partial differential equations in multiple dimensions, such as Eulers equations and the compressible Navier-Stokes equations, using Discontinuous Galerkin [8] spectral element spatial discretizations.

2D Nozzle Flow and Conclusion:

The three-dimensional Navier-Stokes (NS) equations describe the behavior of many types of fluids and are given below:

$$\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho w\\ E\end{bmatrix}_t+\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ \rho uw\\ (E+p)u\end{bmatrix}_x+\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ \rho vw\\ (E+p)v\end{bmatrix}_y+\begin{bmatrix}\rho w\\ \rho uw\\ \rho vw\\ \rho w^2+p\\ (E+p)w\end{bmatrix}_z=$$

$$\frac{1}{Re}\left(\begin{bmatrix}0\\ \tau_{xx}\\ \tau_{yx}\\ \tau_{zx}\\ \tau_{xx}u+\tau_{yx}v+\tau_{zx}w+\frac{\gamma k}{Pr}\frac{\partial T}{\partial x}\end{bmatrix}_x+\begin{bmatrix}0\\ \tau_{xy}\\ \tau_{yy}\\ \tau_{zy}\\ \tau_{xy}u+\tau_{yy}v+\tau_{zy}w+\frac{\gamma k}{Pr}\frac{\partial T}{\partial y}\end{bmatrix}_y+\begin{bmatrix}0\\ \tau_{xz}\\ \tau_{yz}\\ \tau_{zz}\\ \tau_{xz}u+\tau_{yz}v+\tau_{zz}w+\frac{\gamma k}{Pr}\frac{\partial T}{\partial z}\end{bmatrix}_z\right)$$

$Re=\frac{\rho uL}{\mu}=$ Reynolds number, $Pr=\frac{c_p\mu}{k}$, $E=\rho\left(T+\frac{1}{2}\left(u^2+v^2+w^2\right)\right)=$ total energy,

$\mu=$ dynamic viscosity, $\lambda=$ bulk viscosity, $k=$ coefficient of thermal conductivity,

stress tensor elements: $\tau_{x_i x_j}=\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)+\delta_{ij}\lambda\sum\frac{\partial u_k}{\partial x_k}$, $\delta_{ij}=$ Kronecker delta,

$\gamma=\frac{c_p}{c_v}=\frac{\text{heat capacity (constant pressure)}}{\text{heat capacity (constant volume)}}$

For our test case, we solve the two-dimensional Euler equations (in a nozzle), which can be derived from the NS equations by taking the limit of Reynolds number going to infinity (right-hand side in above equations becomes 0).

The axisymmetric converging-diverging nozzle has area given by:

$$\text{Area}(x) = 1.75 - .75 * \cos((.2 * x - 1.0) * \text{pi}), \qquad 0 \le x \le 5.0$$

$$\text{Area}(x) = 1.25 - .25 * \cos((.2 * x - 1.0) * \text{pi}), \quad 5.0 \le x \le 10.0$$

We solve a steady-state (SS) problem where the SS solution has a shock at x = 7.56. The inflow Mach number = .240 and the outflow Mach number = .501. The test case until the physical time t = 5, which is well before the time the shock develops. So for our test, the solution is relatively smooth and does not contain shocks, although it does contain some complex structures.

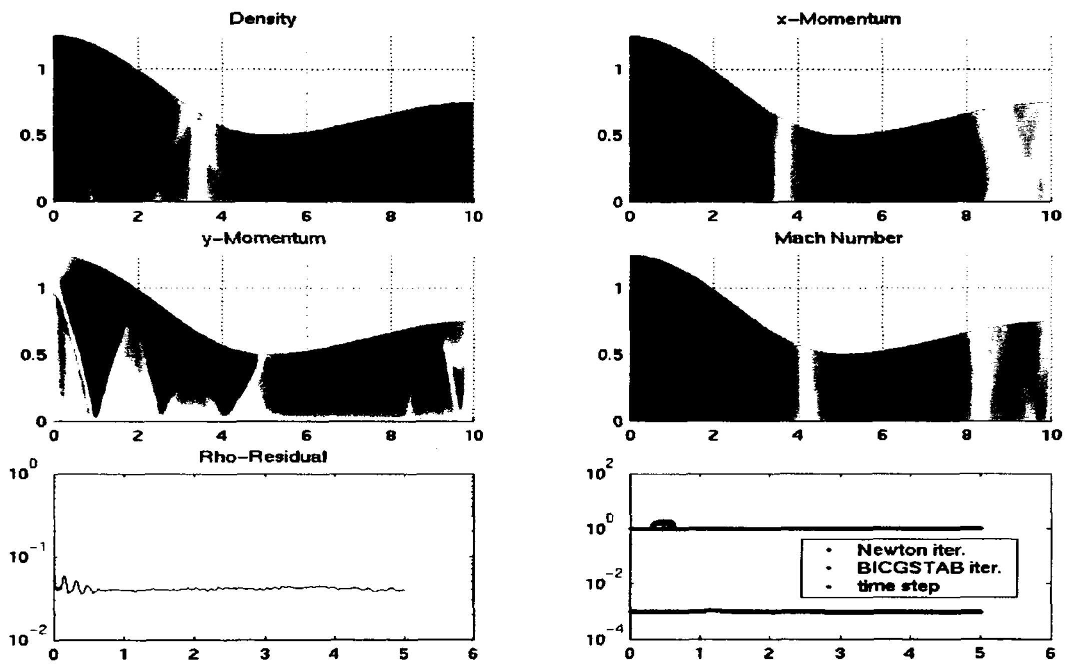

Figure 1: IMEX, N=8, No Preconditioning, Newton Tol. = 1e–3, Bicgstab, Failed=0, nozzle52, CPU–time=11,115s (5,194 time steps)

The implicit elements are located within a semicircular region of radius r = .25 centered at x = 7.562 (center lies on bottom wall/centerline, see figure). The geometric stiffness, which is defined as the ratio of average IMEX time step to average explicit time step is approximately 2.27 (N = 8) for the unstructured triangular mesh used. The ratio of implicit to total elements is 56/496, which is slightly greater than 10%.

We use the method of lines to discretize the partial differential equations in space and time. First, we discretize space using a nodal Discontinuous Galerkin Spectral Element method based on [8]. Next, we integrate the system of ordinary differential equations (ODEs) in time. For the IMEX method, we use a modified Newton-Krylov method (Newton tolerance = 1E-03) to linearize the nonlinear system of ODEs, and to iteratively solve the linear systems (BiCGStab). Both time-integration methods are globally 4^{th}-order accurate. Preconditioners were not used.

We impose boundary conditions on the characteristic variables at the inflow and outflow, and penalize the velocity against its mirror image at the top and bottom walls.

We use a stability time-step controller for all runs:

$\Delta t = CFL/(\lambda * N^2 * \text{geometric factor})$, where λ is the maximum wave speed.

We can see that for N = 8 both methods take approximately the same CPU-time, with the IMEX being slightly faster. For N = 4, the explicit method is faster.

Time-Integration Method	**Polynomial Order (N)**	**Average Time-Step (Δt)**	**Total Time-Steps**	**Total CPU-time (sec.)**
Purely Explicit	4	1.39E-03	3,601	1,349
	8	4.24E-04	11,800	11,313
IMEX	4	3.34E-03	1,499	1,864
	8	9.63E-04	5,194	11,115

IMEX methods are not faster in this particular test, but will be significantly faster for the following situation:

(1) Ratio of implicit to total elements < 5-10%.
(2) Effective Preconditioners.
(3) Geometric Stiffness > 2.
(4) Navier Stokes equations, which have viscous terms.
(5) Advanced Time-Step Controller (PID).

We believe that when some or all of the above are implemented, IMEX methods will become significantly more efficient than purely explicit time-integration methods.

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