# REPORT DOCUMENTATION PAGE

*Form Approved*
*OMB No. 0704-0188*



**1. REPORT DATE** *(DD-MM-YYYY)*
February 1, 2012

**2. REPORT TYPE**
Final Performance Report

**3. DATES COVERED** *(From - To)*
03/01/2009-11/30/2011

**4. TITLE AND SUBTITLE**
HIGH ORDER STRONG STABILITY PRESERVING TIME DISCRETIZATIONS FOR THE TIME EVOLUTION OF HYPERBOLIC PARTIAL DIFFERENTIAL EQUATIONS

**5a. CONTRACT NUMBER**
FA9550-09-1-0208

**5b. GRANT NUMBER**

**5c. PROGRAM ELEMENT NUMBER**

**6. AUTHOR(S)**
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**5d. PROJECT NUMBER**

**5e. TASK NUMBER**

**5f. WORK UNIT NUMBER**

**7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)**

U. of Massachusetts Dartmouth
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North Dartmouth MA 02747

**8. PERFORMING ORGANIZATION REPORT NUMBER**

**9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)**
AFOSR
875 N. Randolph St.
Suite 325
Arlington, VA 22203

**10. SPONSOR/MONITOR'S ACRONYM(S)**

**11. SPONSOR/MONITOR'S REPORT NUMBER(S)**
AFRL-OSR-VA-TR-2012-0390

**12. DISTRIBUTION / AVAILABILITY STATEMENT**

A

**13. SUPPLEMENTARY NOTES**

**14. ABSTRACT**
The objective of this project is to develop and analyze stable time discretizations suitable for the simulation of hyperbolic time-dependent partial differential equations. Implicit and explicit multi-step multi-stage time discretizations with optimal time-step restrictions have been developed, as well as implicit Runge--Kutta methods with downwinding and unconditional stability. A testing suite has been written to test some of these methods with a variety of spatial discretizations. New directions have been explored for implicit-explicit methods, which are useful for problems with convection and diffusion. Finally, novel provably stable multi-step time discretizations for use with Fourier pseudo-spectral spatial approximations of the three dimensional viscous Burgers' equations and Navier-Stokes equations have been developed.

**15. SUBJECT TERMS**
strong stability preserving methods, time discretizations, hyperbolic partial differential equations, Runge—Kutta methods, multistep methods, implicit-explicit methods

| 16. SECURITY CLASSIFICATION OF: | | | 17. LIMITATION OF ABSTRACT | 18. NUMBER OF PAGES | 19a. NAME OF RESPONSIBLE PERSON |
|---|---|---|---|---|---|
| a. REPORT | b. ABSTRACT | c. THIS PAGE | | | Sigal Gottlieb |
| U | U | U | UU | 7 | 19b. TELEPHONE NUMBER *(include area code)* 401-339-5010 |

# Final Report
# Grant/Contract Title: HIGH ORDER STRONG STABILITY PRESERVING TIME DISCRETIZATIONS FOR THE TIME EVOLUTION OF HYPERBOLIC PARTIAL DIFFERENTIAL EQUATIONS
# Grant Number: FA9550-09-1-0208

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## 1 Abstract

The objective of this project is to develop and analyze stable time discretizations suitable for the simulation of hyperbolic time-dependent partial differential equations. Implicit and explicit multi-step multi-stage time discretizations with optimal time-step restrictions have been developed, as well as implicit Runge–Kutta methods with downwinding and unconditional stability. New directions have been explored for implicit-explicit methods, which are useful for problems with convection and diffusion. Finally, novel provably stable multi-step time discretizations for use with Fourier pseudo-spectral spatial approximations of the three dimensional viscous Burgers equations and Navier-Stokes equations have been developed.

## 2 Summary

In this second year of the grant, I have made progress in three directions. First, we developed optimization codes that search for implicit and explicit multi-stage multistep methods of more than two steps. These codes are now being utilized to find three step Runge–Kutta methods with optimal SSP coefficients. Next, we have made significant progress in developing Runge–Kutta methods with downwinding and unlimited time-step, as well as testing appropriate boundary conditions for such methods. We investigated implicit-explicit methods with interesting SSP properties, a promising direction we intend to continue to develop. Finally, we have developed a series of multistep methods which are provably stable for use with Fourier pseudospectral spatial discretizations of 3D viscous Burgers' equation and the 3D Navier-Stokes equations. Also in this year, we published a book on SSP time discretization methods.

## 3 Objectives and accomplishments

1. **Objective: Study the class of high order implicit and explicit SSP Runge-Kutta methods with downwinding to allow for higher order SSP methods.**

   *Motivation:* To more easily analyze SSP methods, we rewrite Runge–Kutta methods in the form:

$$
\begin{aligned}
u^{(0)} &= u^n, \\
u^{(i)} &= \sum_{k=0}^{i-1} \left( \alpha_{i,k} u^{(k)} + \Delta t \beta_{i,k} F(u^{(k)}) \right), \quad \alpha_{i,k} \geq 0, \qquad i = 1, ..., m
\end{aligned}
\tag{3.1}
$$

$$u^{n+1} = u^{(m)}.$$

Explicit SSP Runge-Kutta methods are known to be limited to fourth order and implicit SSP Runge-Kutta methods are limited to sixth order. However, if we allow the use of negative coefficients $\beta_{i,k}$ it is possible to overcome this order barrier. The presence of negative coefficients requires the use of a modified spatial discretization for these instances. When $\beta_{i,k}$ is negative, $\beta_{i,k}F(u^{(k)})$ is replaced by $\beta_{i,k}\tilde{F}(u^{(k)})$, where $\tilde{F}$ approximates the same spatial derivative(s) as $F$, but the strong stability property holds for the first order Euler scheme, solved backward in time. Numerically, the only difference is the change of the upwind direction.

The order barrier on explicit SSP Runge–Kutta methods, and the bounds on the SSP coefficient for implicit SSP Runge–Kutta methods, leave no efficient options for methods of order five and above. This gap may be filled by explicit and implicit SSP Runge–Kutta methods with downwinding.

*Accomplishments:*

(a) I have created an optimization code in MATLAB which seeks implicit methods with downwinding with a large allowable SSP coefficient.

(b) The code has been re-written in Python to facilitate open source reproduction of results

(c) This code has produced results for implicit methods of orders 2-4, and in future will produce higher order methods

(d) A similar optimization code has been developed for explicit methods and for diagonally implicit methods.

(e) These methods have been tested on a test suite of specially selected of problems.

2. **Objective: Study classes of high order implicit and explicit general linear methods to find SSP methods with optimal time-step restrictions.**

*Motivation:* Without the use of *downwinding*, explicit SSP Runge-Kutta methods are limited to fourth order and implicit SSP Runge-Kutta methods are limited to sixth order. SSP multistep methods do not suffer from this order barrier, but have very restrictive SSP coefficients. Efficient explicit SSP methods of order greater than four are frequently desirable, particularly when dealing with high order spatial discretizations. General linear methods, which have multiple steps and multiple stages have the potential to combine the properties of multistep and Runge–Kutta methods, and so provide an advantage over these methods by allowing a larger step-size [4, 3]. We have shown [1] that explicit general linear methods have a bound on the SSP coefficient which is equal to the number of stages. Even considering this bound, explicit general linear methods may be found that have order $p > 4$ and larger SSP coefficient than the multistep methods. A first effort in this direction has been made by [2], which considered a subset of general linear methods.

Multistep Runge-Kutta methods are a straightforward generalization of Runge-Kutta and linear multistep methods, and take the form

$$\begin{aligned} y_i^n &= \textstyle\sum_{j=1}^k d_{ij} u^{n+1-j} + \Delta t \sum_{j=1}^s a_{ij} f(y_j^n), \quad 1 \le i \le s, \\ u^{n+1} &= \textstyle\sum_{j=1}^k \theta_j u^{n+1-j} + \Delta t \sum_{j=1}^s b_j f(y_j^n). \end{aligned}$$

Here the values $u^n$ denote solution values at the times $t = n\Delta t$, while the values $y_j^n$ are intermediate stages used to compute the next solution value. We will also consider a simple generalization of these methods, based on the following reasoning. For some methods, it may happen that the row $i$ of $A$ is identically zero and row $i$ of $D$ is $(1, 0, \ldots, 0)$, so that $y_1^n = u^n$. Then the method involves $f(u^n)$, and at any step we will have computed already $f(u^{n+1-j})$ for $j = 1, \ldots, k$, so these values may as well be used in computing the next step. This leads to methods of the form

$$\begin{array}{ll} y_1^n & = u^n, \\ y_i^n & = \sum_{j=1}^k d_{ij} u^{n+1-j} + \Delta t \sum_{j=2}^k \hat{a}_{ij} f(u^{n+1-j}) + \Delta t \sum_{j=1}^s a_{ij} f(y_j^n), \quad 2 \le i \le s, \\ u^{n+1} & = \sum_{j=1}^k \theta_j u^{n+1-j} + \Delta t \sum_{j=2}^k \hat{b}_j f(u^{n+1-j}) + \Delta t \sum_{j=1}^s b_j f(y_j^n). \end{array}$$

This form is more suitable for finding explicit methods.

*Accomplishments:*

(a) We have found high order (up to 9th) explicit SSP RK methods with large effective SSP coefficients among the class of 2-step RK methods. The paper has been published.

(b) We currently have a code running to numerically find optimal high order implicit SSP multistep RK methods with more than 2 steps. We have verified numerically that the optimal methods are all one-step diagonally implicit methods with $c = 2$. The paper is in preparation.

(c) We modified the above code running for diagonally implicit SSP multistep RK methods with more than 2 steps, and will be running it next.

(d) We modified the above code running for explicit SSP multistep RK methods with more than 2 steps using second form above. The code has produced optimal methods up to order 6 and is currently working on methods of orders 7-10. The paper is in preparation.

3. **Objective: Study possibilities for efficient implicit-explicit SSP methods.** Frequently we are faced with problems of the type

$$u^{n+1} = u^n + \Delta t F(u^n) + \Delta t G(u^{n+1})$$

which are unconditionally stable, but only first order. Because higher order implicit methods (without downwinding) cannot be unconditionally unstable, we cannot extend this to higher order.

However, if we are given a different type of method, one for which

$$u^{n+1} = u^n + \Delta t F(u^n) + \Delta t^k G(u^{n+1})$$

is provably unconditionally stable, then we can develop SSP methods which are higher order and unconditionally SSP.

*Accomplishments:*

(a) The observation above is an accomplishment – it changes the usual paradigm for looking at IMEX methods.

(b) We have applied this idea to problems with artificial viscosity in spectral methods

4. **Objective: Tailor semi-implicit methods for the stable solution of the 3D viscous Burgers' equation and the Navier-Stokes equations**

*Motivation:* We consider the three-dimensional viscous Burgers' equation with periodic boundary conditions,

$$\partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} = \nu\Delta\boldsymbol{u}, \tag{3.2}$$

where $\boldsymbol{u} = (u, v, w)^T$ is the velocity field in the $x$, $y$, and $z$ directions, and $\nu > 0$ is the viscosity. We discretize the spatial terms using a Fourier collocation (pseudospectral) method, and the time-derivative using a variety of suitably chosen semi-implicit multistep methods. Although this method has been widely applied to this problem (and the similar problem of the Navier-Stokes equations), a fully-discrete stability analysis has not been performed. Moreover, it is not clear what time-stepping is stable.

We begin with a first-order in time method which treats the nonlinear convection term explicitly for the sake of numerical convenience, and the diffusion term implicitly to avoid a severe time-step restriction:

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + \boldsymbol{u}^n\cdot\nabla_N\boldsymbol{u}^n = \nu\Delta_N\boldsymbol{u}^{n+1}, \tag{3.3}$$

where, for example, the first component of the nonlinear convection is

$$\boldsymbol{u}^n\cdot\nabla_N u^n = u^n\mathcal{D}_{Nx}u^n + v^n\mathcal{D}_{Ny}u^n + w^n\mathcal{D}_{Nz}u^n.$$

In our recent paper, we performed a fully-discrete analysis and found that this method is unconditionally stable for any final time $T^*$ provided that the time step $\Delta t$ and the space grid size $h$ are bounded by given constants

$$\Delta t \leq L_1(T^*, \nu), \quad h \leq L_2(T^*, \nu).$$

These convergence constants depend on the exact solution, as well as $T^*$ and $\nu$.

If desired, we could use a fully explicit method and prove stability for a time-step restriction of the form $\Delta t \leq C\Delta x^2$, at which point we could apply an SSP method up to fourth order and maintain the stability of this method. However, if we wish to avoid this approach we need to tailor the time-discretizations. (This is due to the problem that IMEX methods do not maintain the SSP property, as mentioned above).

*Accomplishments:*

(a) *We derived a provably stable second order scheme for the 3D Burgers' equation.* For the convection term we use a standard second order Adams-Bashforth extrapolation formula, which involves the numerical solutions at time node points $t^n$, $t^{n-1}$, with well-known coefficients $3/2$ and $-1/2$, respectively. The diffusion term is treated implicitly, using a second order Adams-Moulton interpolation. Treating the diffusion term with a standard second order Adams-Moulton formula leads to a Crank-Nicolson scheme, which gives us difficulties in the stability analysis.

Instead, we look for an Adams-Moulton interpolation such that the diffusion term is more focused on the time step $t^{n+1}$, i.e., the coefficient at time step $t^{n+1}$ dominates the sum of all other diffusion coefficients. We discovered that the Adams-Moulton interpolation which involves the time node points $t^{n+1}$ and $t^{n-1}$ gives the corresponding coefficients as $3/4$, $1/4$, respectively, which satisfies the unconditional stability condition. Therefore, we formulate the fully discrete scheme:

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + \frac{3}{2}\boldsymbol{u}^n\cdot\nabla_N\boldsymbol{u}^n - \frac{1}{2}\boldsymbol{u}^{n-1}\cdot\nabla_N\boldsymbol{u}^{n-1} = \nu\Delta_N\left(\frac{3}{4}\boldsymbol{u}^{n+1} + \frac{1}{4}\boldsymbol{u}^{n-1}\right). \tag{3.4}$$

This scheme is provably stable in the same way as the first order scheme.

(b) *We derived provably stable third and fourth order schemes for the 3D Burgers' equation.* Using similar ideas we derived third and fourth order in time schemes for (3.2). The nonlinear convection term is updated by an explicit Adams-Bashforth extrapolation formula, with the time node points $t^n$, $t^{n-1}$, ..., $t^{n-k+1}$ involved and an order of accuracy $k$. The diffusion term is computed by an implicit Adams-Moulton interpolation with the given accuracy order in time. To ensure unconditional numerical stability for a fixed time, we have to derive an Adams-Moulton formula such that the coefficient at time step $t^{n+1}$ dominates the sum of the other diffusion coefficients. In more detail, a $k$-th order (in time) scheme takes the form of

$$\frac{\boldsymbol{u}^{n+1}-\boldsymbol{u}^n}{\Delta t}+\sum_{i=0}^{k-1} B_i \boldsymbol{u}^n \cdot \nabla_N \boldsymbol{u}^{n-i}=\nu \Delta_N\left(D_0 \boldsymbol{u}^{n+1}+\sum_{i=0}^{k-1} D_{j(i)} \boldsymbol{u}^{n-j(i)}\right). \tag{3.5}$$

in which $B_i \mid_{i=0}^{k-1}$ are the standard Adams-Bashforth coefficients with extrapolation points $t^n$, $t^{n-1}$, ..., $t^{n-k+1}$, $j(i) \mid_{i=0}^{k-1}$ are a set of (distinct) indices with $j(i) \geq 0$, and $D_0$, $D_{j(i)} \mid_{i=0}^{k-1}$ correspond to the Adams-Moulton coefficients to achieve the $k$-th order accuracy. Moreover, a necessary condition for unconditional numerical stability is given by

$$D_0>\sum_{i=0}^{k-1}\left|D_{j(i)}\right|. \tag{3.6}$$

To derive an Adams-Moulton formula for the diffusion term, whose coefficients satisfy the condition (3.6), we require a stretched stencil. In particular, for the third order scheme, it can be shown that a stencil comprised of the node points $t^{n+1}$, $t^{n-1}$ and $t^{n-3}$ is adequate. The fully discrete scheme can be formulated as:

$$\begin{aligned} & \frac{\boldsymbol{u}^{n+1}-\boldsymbol{u}^n}{\Delta t}+\frac{23}{12} \boldsymbol{u}^n \cdot \nabla_N \boldsymbol{u}^n-\frac{4}{3} \boldsymbol{u}^{n-1} \cdot \nabla_N \boldsymbol{u}^{n-1}+\frac{5}{12} \boldsymbol{u}^{n-2} \cdot \nabla_N \boldsymbol{u}^{n-2} \\ = & \nu \Delta_N\left(\frac{2}{3} \boldsymbol{u}^{n+1}+\frac{5}{12} \boldsymbol{u}^{n-1}-\frac{1}{12} \boldsymbol{u}^{n-3}\right). \end{aligned} \tag{3.7}$$

For the fourth order scheme, we use an Adams-Moulton interpolation at node points $t^{n+1}$, $t^{n-1}$, $t^{n-5}$ and $t^{n-7}$ for the diffusion term. Combined with the Adams-Bashforth extrapolation for the nonlinear convection term, the scheme is given by

$$\begin{aligned} & \frac{\boldsymbol{u}^{n+1}-\boldsymbol{u}^n}{\Delta t}+\frac{55}{24} \boldsymbol{u}^n \cdot \nabla_N \boldsymbol{u}^n-\frac{59}{24} \boldsymbol{u}^{n-1} \cdot \nabla_N \boldsymbol{u}^{n-1}+\frac{37}{24} \boldsymbol{u}^{n-2} \cdot \nabla_N \boldsymbol{u}^{n-2}-\frac{3}{8} \boldsymbol{u}^{n-3} \cdot \nabla_N \boldsymbol{u}^{n-3} \\ = & \nu \Delta_N\left(\frac{757}{1152} \boldsymbol{u}^{n+1}+\frac{470}{1152} \boldsymbol{u}^{n-1}-\frac{118}{1152} \boldsymbol{u}^{n-5}+\frac{43}{1152} \boldsymbol{u}^{n-7}\right). \end{aligned} \tag{3.8}$$

In the third order case, we observe that a direct application of the Adams-Moulton formula at the nodes $t^{n+1}$, $t^n$ and $t^{n-1}$ (corresponding to $j(i)=i$ in the general form (3.5)) does not give a formula with the stated stability property. For example, a "naive" combination of 3rd order Adams-Bashforth for the nonlinear convection and Adams-Moulton for the diffusion term results in the following scheme

$$\begin{aligned} & \frac{\boldsymbol{u}^{n+1}-\boldsymbol{u}^n}{\Delta t}+\frac{23}{12} \boldsymbol{u}^n \cdot \nabla_N \boldsymbol{u}^n-\frac{4}{3} \boldsymbol{u}^{n-1} \cdot \nabla_N \boldsymbol{u}^{n-1}+\frac{5}{12} \boldsymbol{u}^{n-2} \cdot \nabla_N \boldsymbol{u}^{n-2} \\ = & \nu \Delta_N\left(\frac{5}{12} \boldsymbol{u}^{n+1}+\frac{2}{3} \boldsymbol{u}^n-\frac{1}{12} \boldsymbol{u}^{n-1}\right), \end{aligned}$$

which violates the stability condition (3.6). **Moreover, numerical experiments also showed that this method is in fact unstable.** This case highlights the need to choose an appropriate time-discretization to couple with the pseudospectral method.

## 4 Dissemination

We continue to update our SSP RK web-site to disseminate the results of the study. This site serves as an online catalog of all the methods studied, noting which are most successful, and commenting on the theoretical properties of each, and on which performed best with which spatial approximation.

In Summer 2010, I organized two minisymposium sessions on SSP methods at the SIAM annual meeting in Pittsburgh.

A book on SSP methods, written with colleagues David Ketcheson and Chi-Wang Shu was published by World Scientific Press.

**Acknowledgment/Disclaimer** This work was sponsored (in part) by the Air Force Office of Scientific Research, USAF, under grant/contract number FA9550-09-1-0208. T he views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.

## References

[1] S. Gottlieb, D.I. Ketcheson and C.-W. Shu. High Order Strong Stability Preserving Time Discretizations. *Journal of Scientific Computing* , **vol 38**, No. 3 (2009), pp. 251–289.

[2] C. Huang. Strong Stability Preserving Hybrid Methods. *Applied Numerical Mathematics*, doi: 10.1016/j.apnum.2008.03.030, 2008.

[3] D.I. Ketcheson, C.B. Macdonald and S. Gottlieb. Optimal implicit strong stability preserving Runge-Kutta methods. *Applied Numerical Mathematics*, doi: 10.1016/j.apnum.2008.03.034.

[4] H.W.J. Lenferink. Contractivity-preserving implicit linear multistep methods. *Mathematics of Computation*, 56:177–199, 1991.

## Personnel Supported During Duration of Grant

Sigal Gottlieb, Professor of Mathematics, UMass Dartmouth.
Saeja Kim, Associate Professor of Mathematics, UMass Dartmouth.
Zachary Grant, Undergraduate Student, UMass Dartmouth.
Sidafa Conde, Undergraduate Student, UMass Dartmouth.

## Publications

1. S. Gottlieb, F. Tone, C. Wang, X. Wang, and D. Wirosoetisno, Long time stability of a classical efficient scheme for two dimensional Navier-Stokes equations. SIAM Journal on Numerical Analysis (2012) 50, pp. 126-150

2. D.I. Ketcheson, S. Gottlieb, and C. B. Macdonald, Strong stability preserving two-step Runge-Kutta methods. SIAM Journal on Numerical Analysis. (2012) 49, pp. 2618-2639.

3. Sigal Gottlieb and Cheng Wang, Stability and convergence analysis of fully discrete Fourier collocation spectral method for 3-D viscous Burgers' Equation. Submitted to Journal of Scientific Computing

4. Sigal Gottlieb, David Ketcheson and Chi-Wang Shu Strong Stability Preserving Runge Kutta and Multistep Time Discretizations. World Scientific Press. January 2011. ISBN 978-981-4289-26-9

## Honors & Awards Received:

Sigal Gottlieb was awarded a chancellor colloquium series lecture at UMass Dartmouth, which included a $1,000 award.

**AFRL Point of Contact:** Vassilios Kovanis, PhD, Electro-Optics Components Branch Sensors Directorate. Wright Patterson AFB OH. Phone 937-904-9943. Initial contact by email on 3/24/09, talked twice on the phone about the use of SSP time discretization. Arranged to meet in Fall 2009.

**Transitions:** Information about these numerical methods was requested by
Frank Giraldo, (email: fxgirald@nps.edu, Assoc Professor and Assoc Chair for Research, Department of Applied Mathematics, Monterey, CA) on 8/12/08.
Uri Shumlak, (Professor, Aerospace & Energetics Research Program University of Washington, Seattle, WA), who thought that SSP time-discretization may be applicable to his research developing a DG method for the two-fluid plasma model. Sent him this information on 8/18/08.
Marsha Berger, (Computer Science Department, Courant Institute of Mathematical Sciences, New York University) on 8/14/08.
Zhilin Li, Professor, (e-mail: zhilin@math.ncsu.edu, Department of Mathematics, North Carolina State University, Raleigh, NC) used one of these implicit SSPRK schemes for free boundary/moving interface problems. We discussed this by email on 11/1/09.