Implicit-Explicit Formulations for Fluid Mechanics Applications

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Outline

- Definitions
- Background of Research
- Objectives
- Methodology
- Results
- Future plans
- Questions

Temporal Integrators

Three types of implicit temporal integrators:

- Multistep schemes – Backward Differentiation (BDF)
  - A-stability (L-stable) for 1st and 2nd order only
- Multistage schemes – Runge-Kutta (RK)
  - A-stability at any order, multiple stages increase cost
  - Downside: low stage order $\rightarrow$ order reduction for stiff problems
- General linear methods – mixtures of multistage/multistage (MEBDF4)
  - Extremely hard to design, not very mature

Stiffness

Definitions of Stiffness:

1)Necessitates implicit method for efficiency

2)Separation of temporal scales

- Not interested in high frequency scales
- Use implicit method to jump over high frequency scales

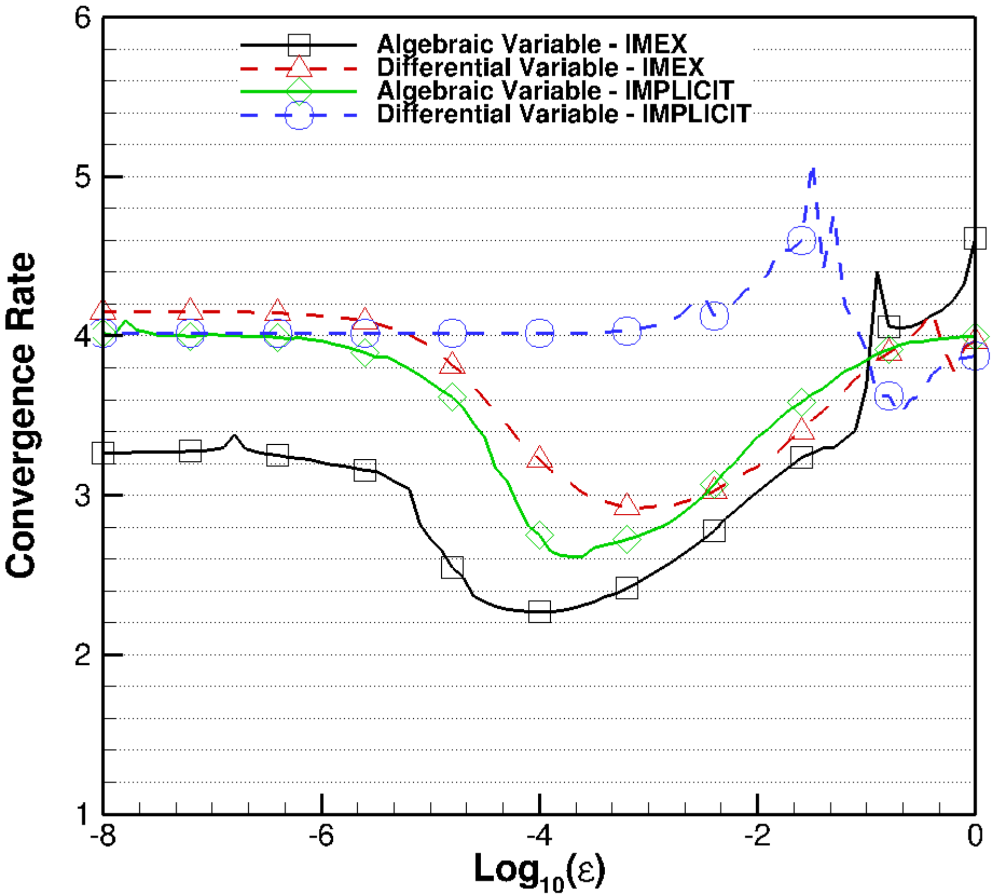
Separable stiffness:

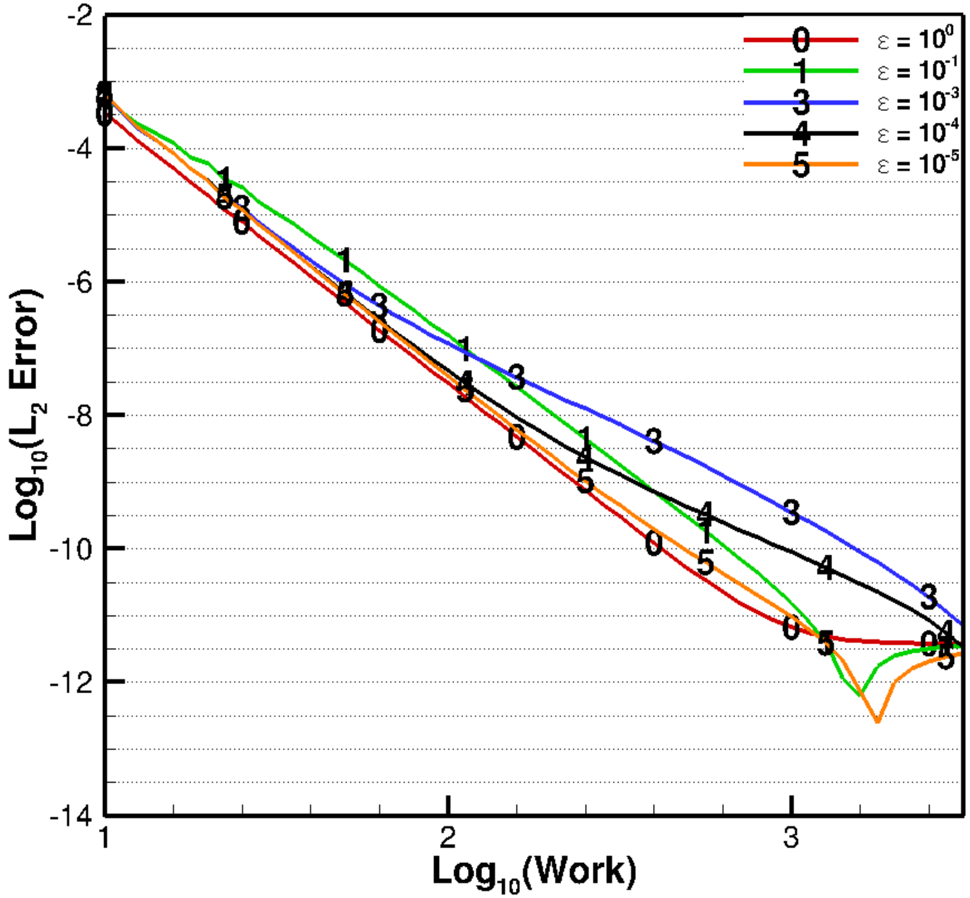
- Form of stiffness where a splitting of the equations is easily identified to isolate the stiffness

Order Reduction

- Specific to multistage schemes, e.g. Runge-Kutta
- Multiple orders: design order, stage order
- Stage order is different between implicit (2) and explicit (1)
- Convergence rate for smooth variables is design order
- Convergence rate for stiff variables is ε*(stage order)

Order Reduction

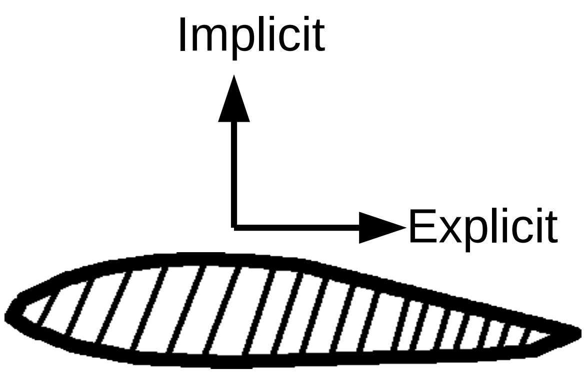




Order reduction for Kaps Problem with ARK436[2]SA_4 RK scheme can be seen at $\varepsilon \approx 10^{-4}$

Background of Research

- Implicit-Explicit RK (IMEX) schemes are optimal for applications with separable stiffness
- Spacial dimensions may be separable
- Individual convection, diffusion, reaction terms may be separable



$$u_t = \nabla u + f(u)$$

Objectives

The objectives of this internship were to:

1) Build testing framework to test IMEX formulations

2) Investigate the efficacy of various IMEX RK schemes on multiple test problems

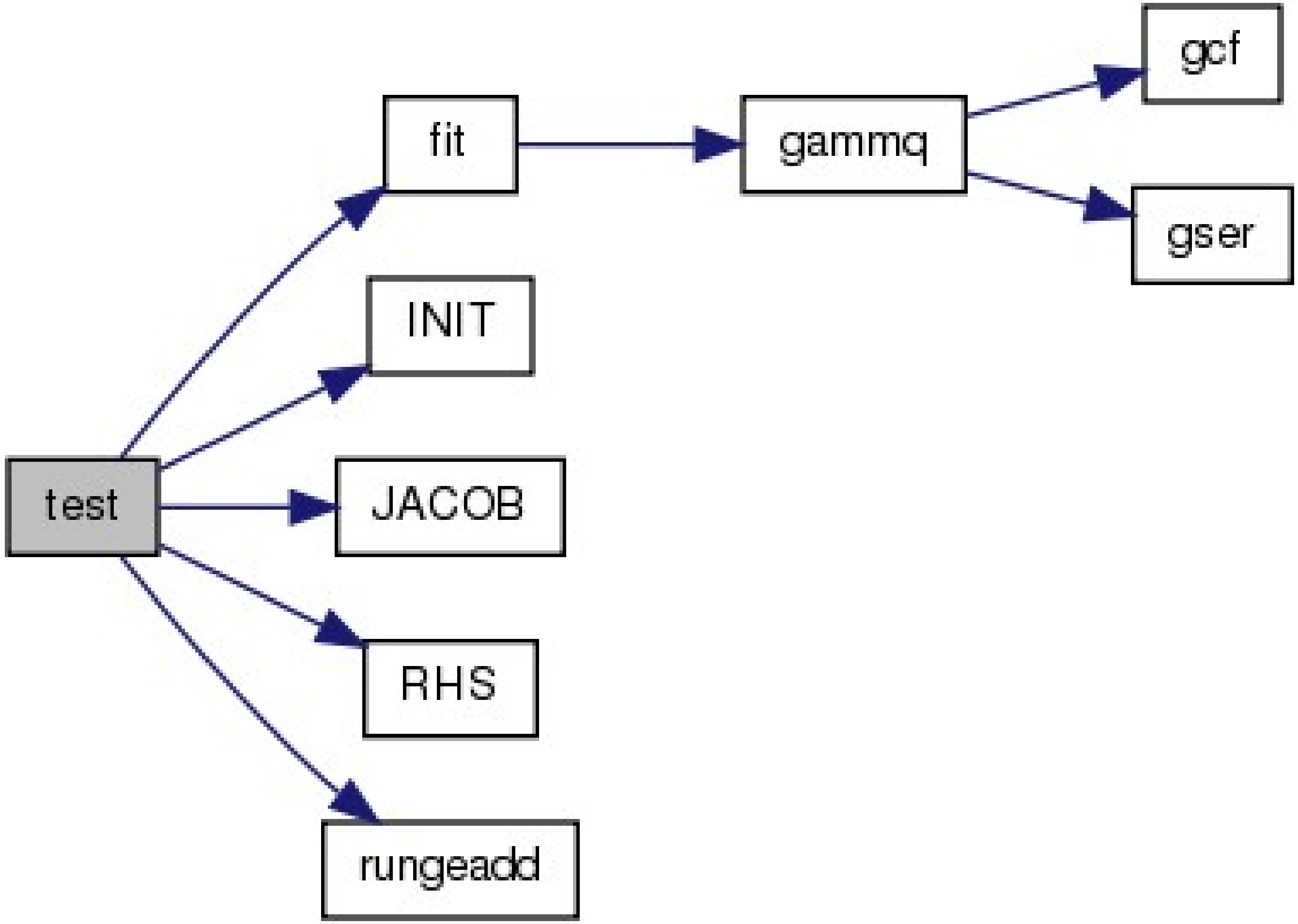
3) Compare convergence rates over varying stiffness of fully Implicit and IMEX formulations

4) Improve schemes from 2003 Applied Numerical Mathematics[1] paper

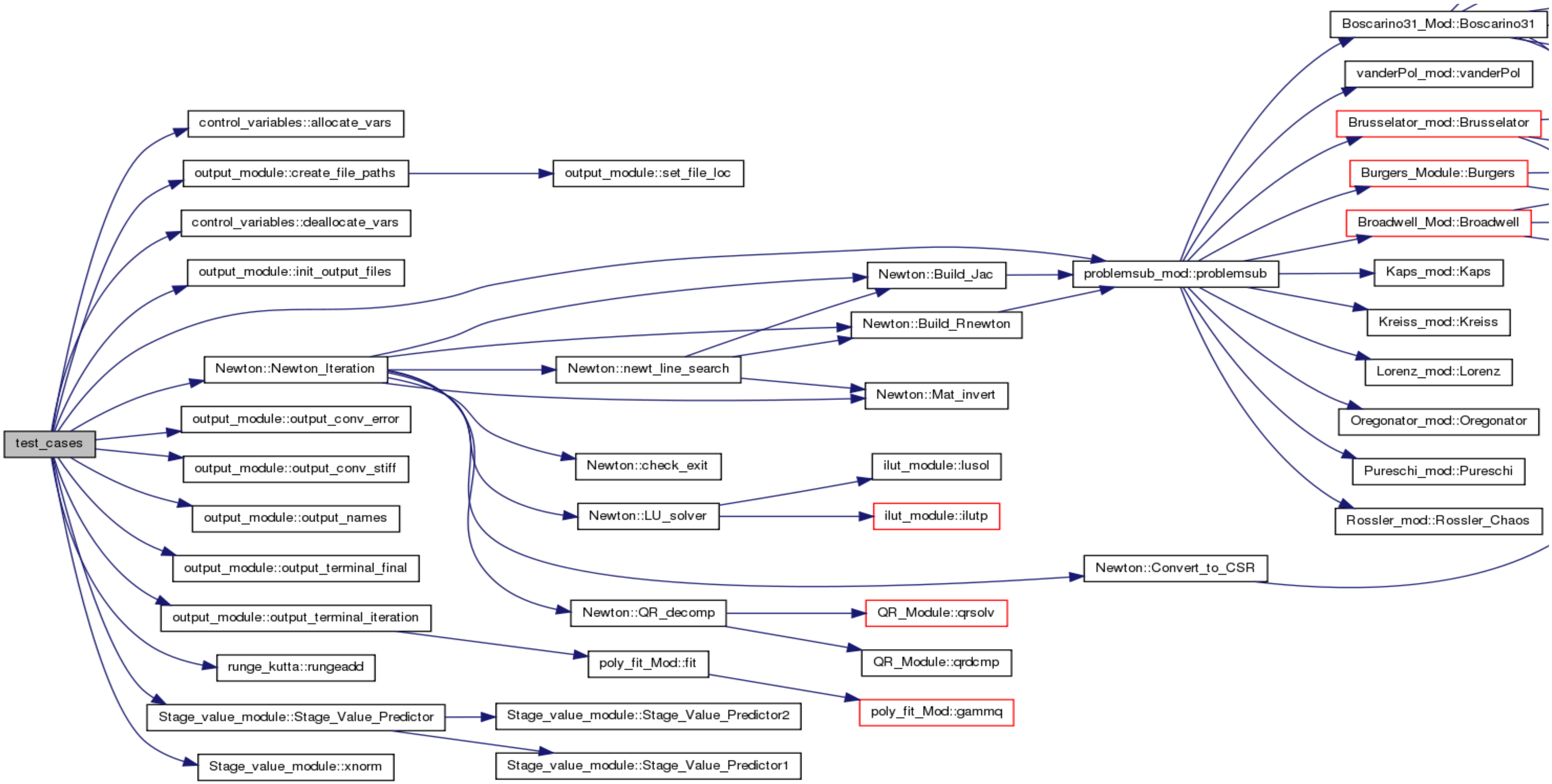
- Decrease order reduction
- Increase diagonal terms to improve convergence of iterative solver

1) Kennedy, Carpenter, “Additive Runge-Kutta schemes for convection-diffusion-reaction equations”. Applied Numerical Mathematics 44 (2003) 139-181.

Test Suite



Test Suite


test_cases
control_variables::allocate_vars
output_module::create_file_paths
output_module::set_file_loc
control_variables::deallocate_vars
output_module::init_output_files
Newton::Newton_Iteration
output_module::output_conv_error
output_module::output_conv_stiff
output_module::output_names
output_module::output_terminal_final
output_module::output_terminal_iteration
runge_kutta::rungeadd
Stage_value_module::Stage_Value_Predictor
Stage_value_module::xnorm
Newton::newt_line_search
Newton::check_exit
Newton::LU_solver
Newton::QR_decomp
poly_fit_Mod::fit
Stage_value_module::Stage_Value_Predictor2
Stage_value_module::Stage_Value_Predictor1
Newton::Build_Jac
Newton::Build_Rnewton
Newton::Mat_invert
ilut_module::lusol
ilut_module::ilutp
QR_Module::qrsolv
QR_Module::qrdcmp
poly_fit_Mod::gammq
problemsub_mod::problemsub
Newton::Convert_to_CSR
Boscarino31_Mod::Boscarino31
vanderPol_mod::vanderPol
Brusselator_mod::Brusselator
Burgers_Module::Burgers
Broadwell_Mod::Broadwell
Kaps_mod::Kaps
Kreiss_mod::Kreiss
Lorenz_mod::Lorenz
Oregonator_mod::Oregonator
Pureschi_mod::Pureschi
Rossler_mod::Rossler_Chaos

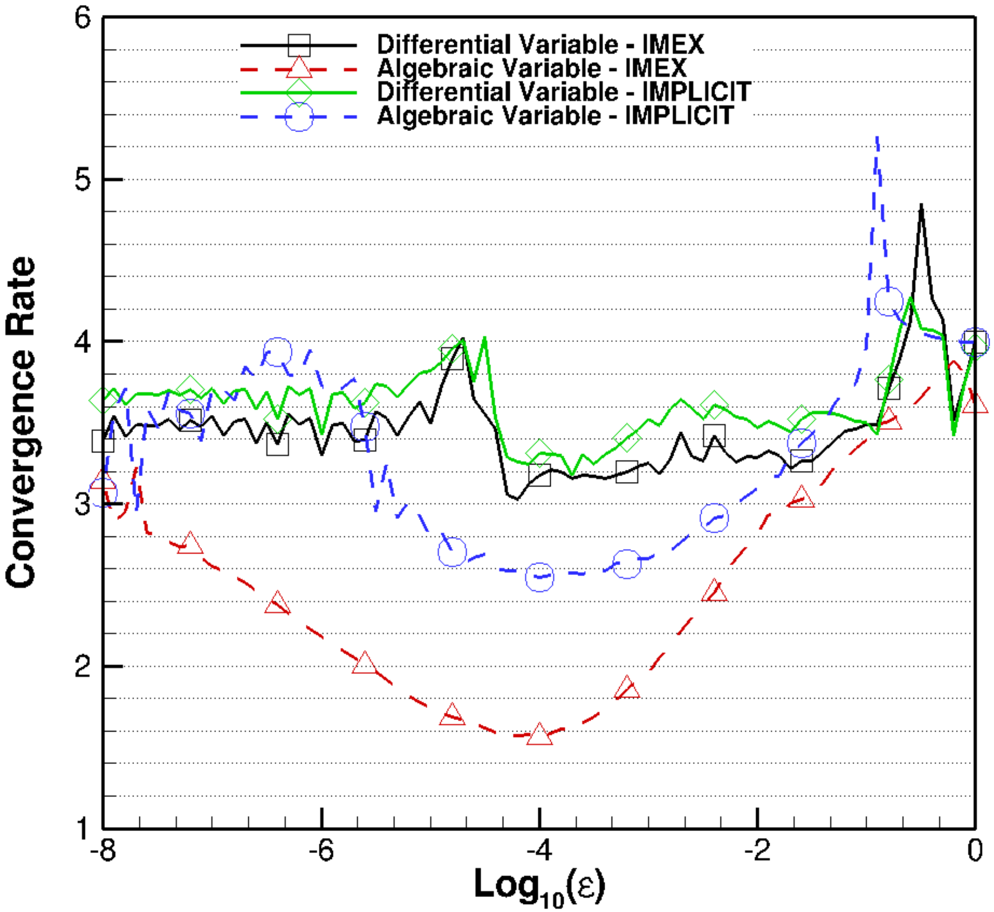
Test Problems

1) Van der Pol (Hairer II, pp. 403)
2) Pureschi and Russo
3) Kaps (Dekker 7.5.2 pp. 215: Index I)
4) Kreiss' (Dekker 7.5.1 pp. 214: Index II)
5) Lorenz Attractor
6) Rossler-Chaos (Wolf, Swift, Swinney, Vastano, Physica 16D, (1985), 285-317)
7) Oregonator
8) Brusselator
9) Burger's Equation
10) Boscarino Eq. 31 (Boscarino, Russo, SIAM J. Sci. Comput., (2009), 1926-1945)
11) Broadwell Model (Boscarino, Russo, SIAM J. Sci. Comput., (2009), 1926-1945)

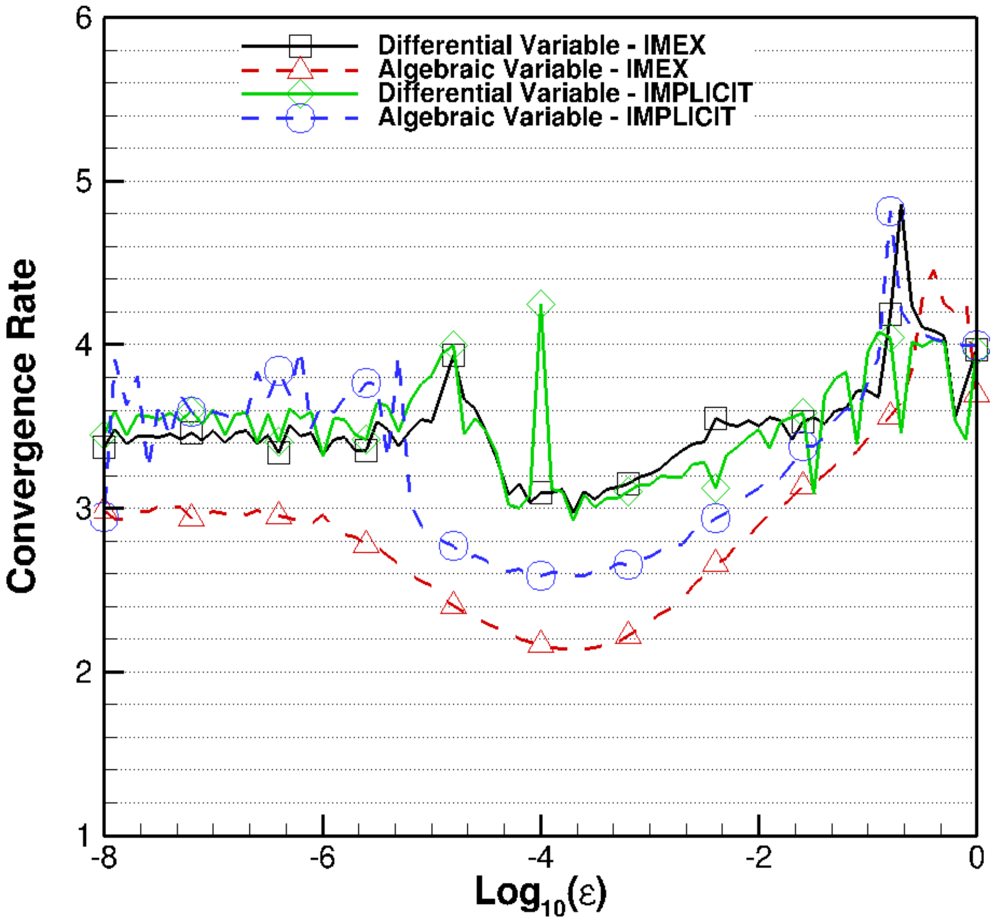
Methodology

- Test problems were selected for their stiffness characteristics
- Compare convergence rates with different stiffness values $10^{-8} \leq \varepsilon \leq 10^{0}$
- Compare error of IMEX formulation against temporal cost with implicit baseline

Order Reduction Improvement: Van der Pol

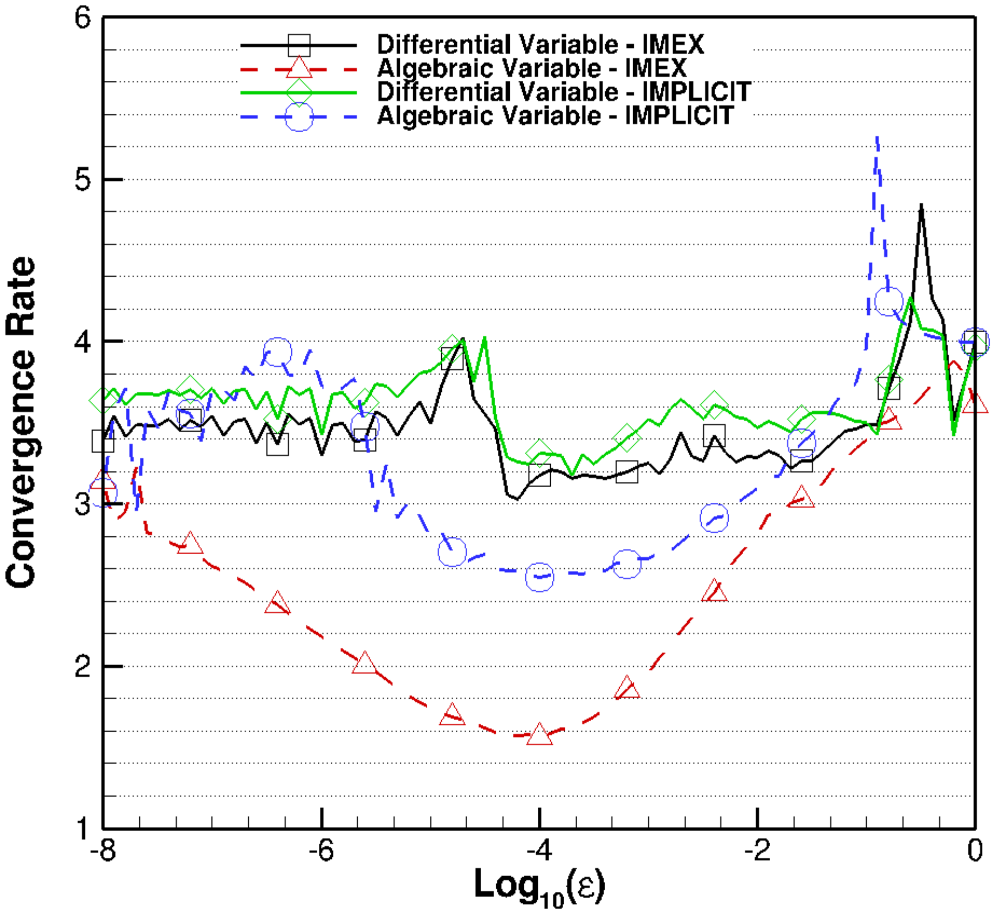


ARK436[2]SA_1

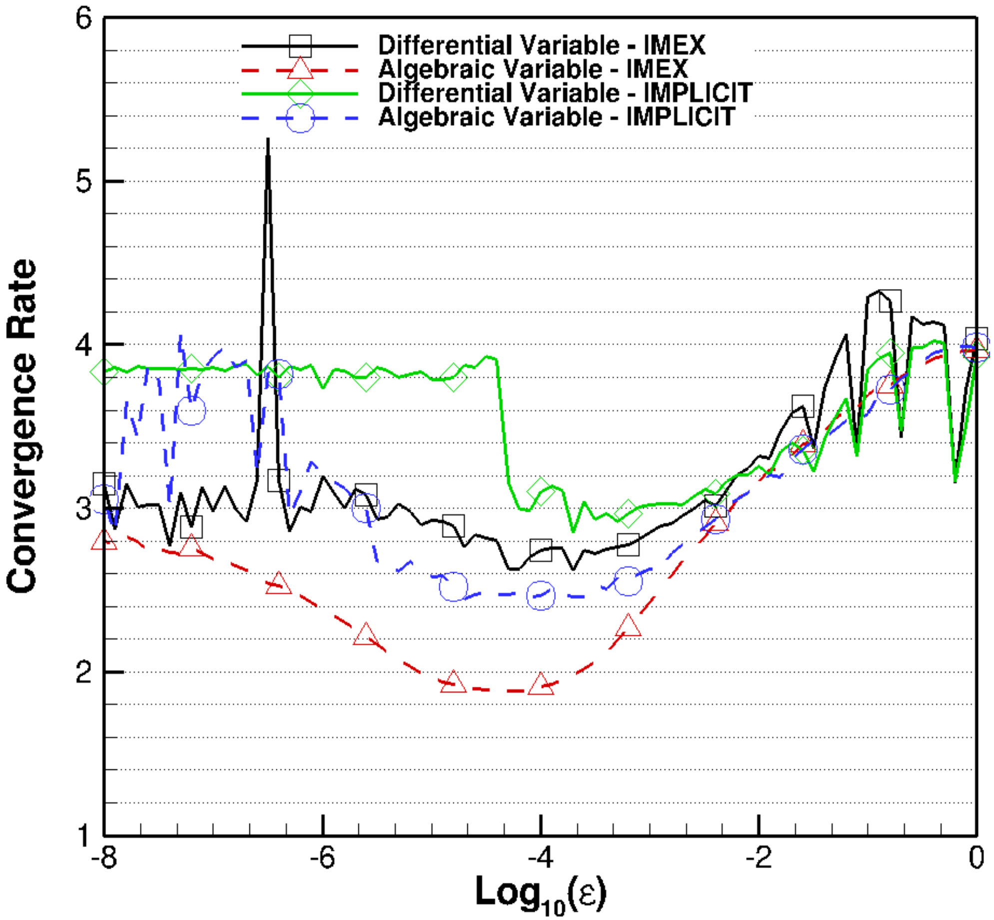


ARK436[2]SA_4

Order Reduction Improvement: Van der Pol

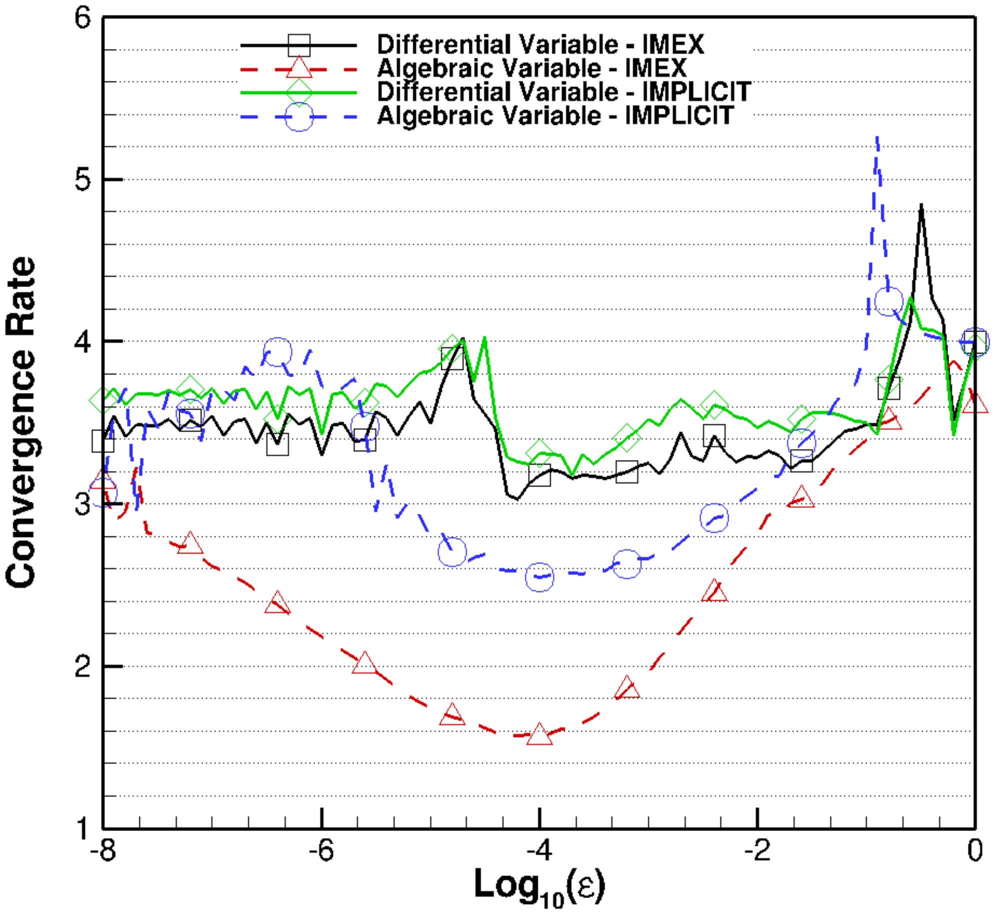


ARK436[2]SA_1

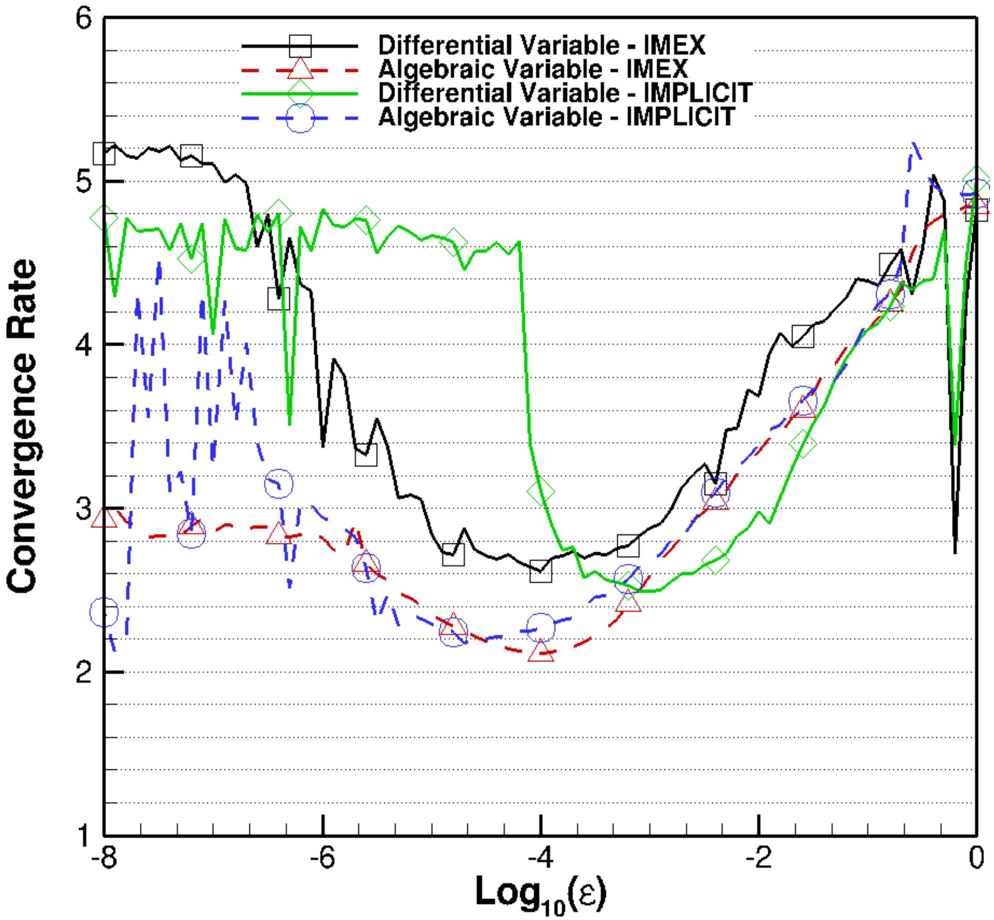


ARK437[2]SA_1 – C2E and C2I

Order Reduction Improvement: Van der Pol



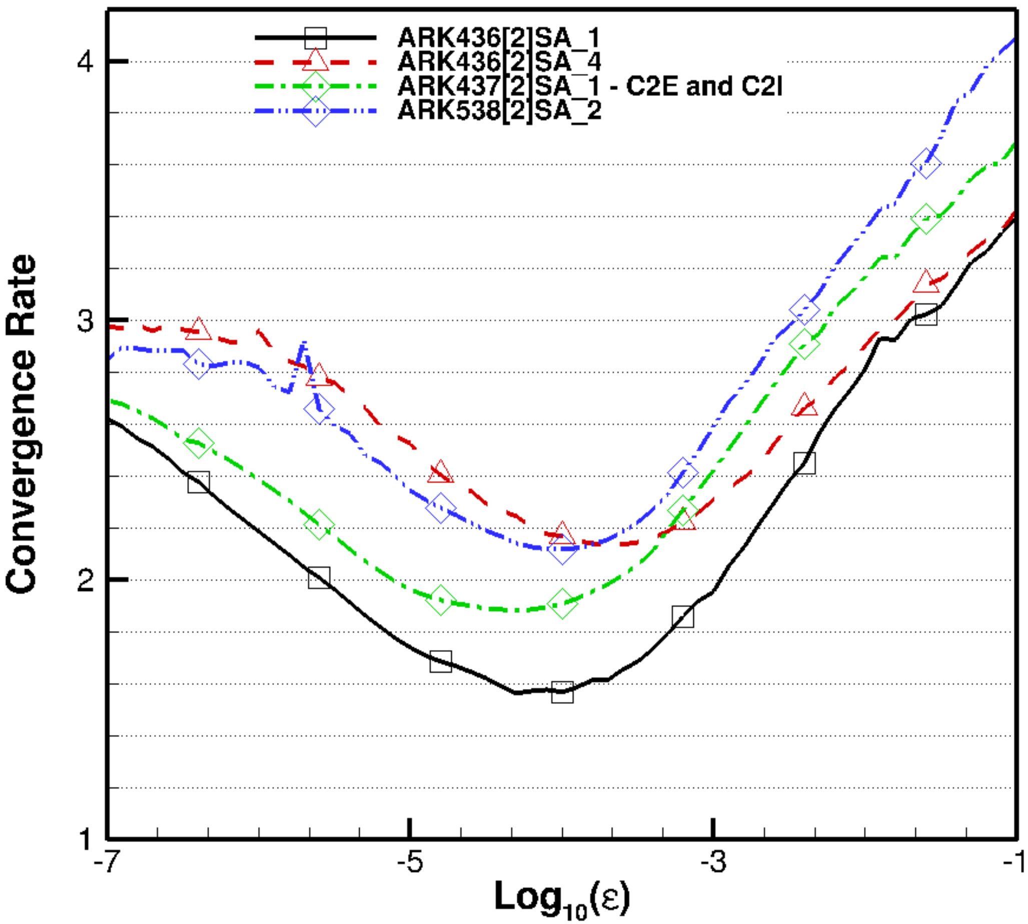
ARK436[2]SA_1



ARK538[2]SA_2

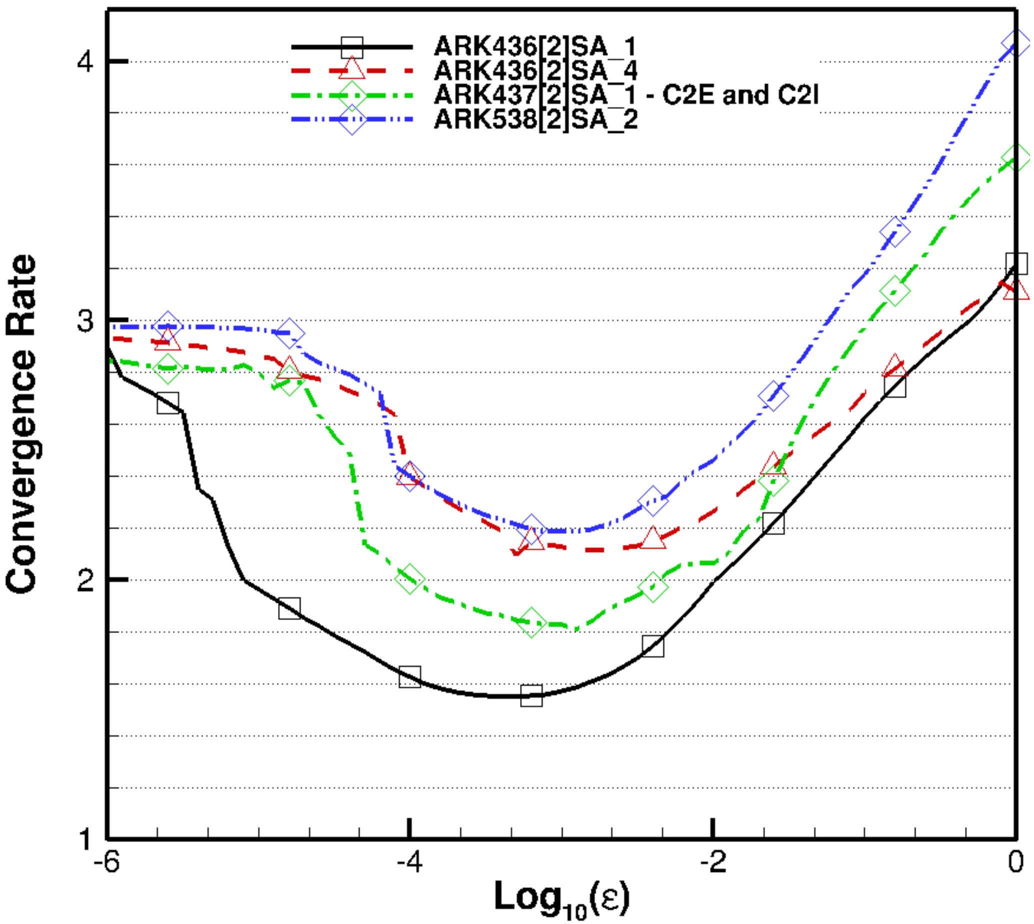
Order Reduction Improvement: Van der Pol

- ARK436[2]SA_1 is baseline scheme
- 5th order ARK538[2]SA_2 and 4th order ARK436[2]SA_4 have similar order reduction
- Multiple schemes on Van der Pol are improvements on baseline



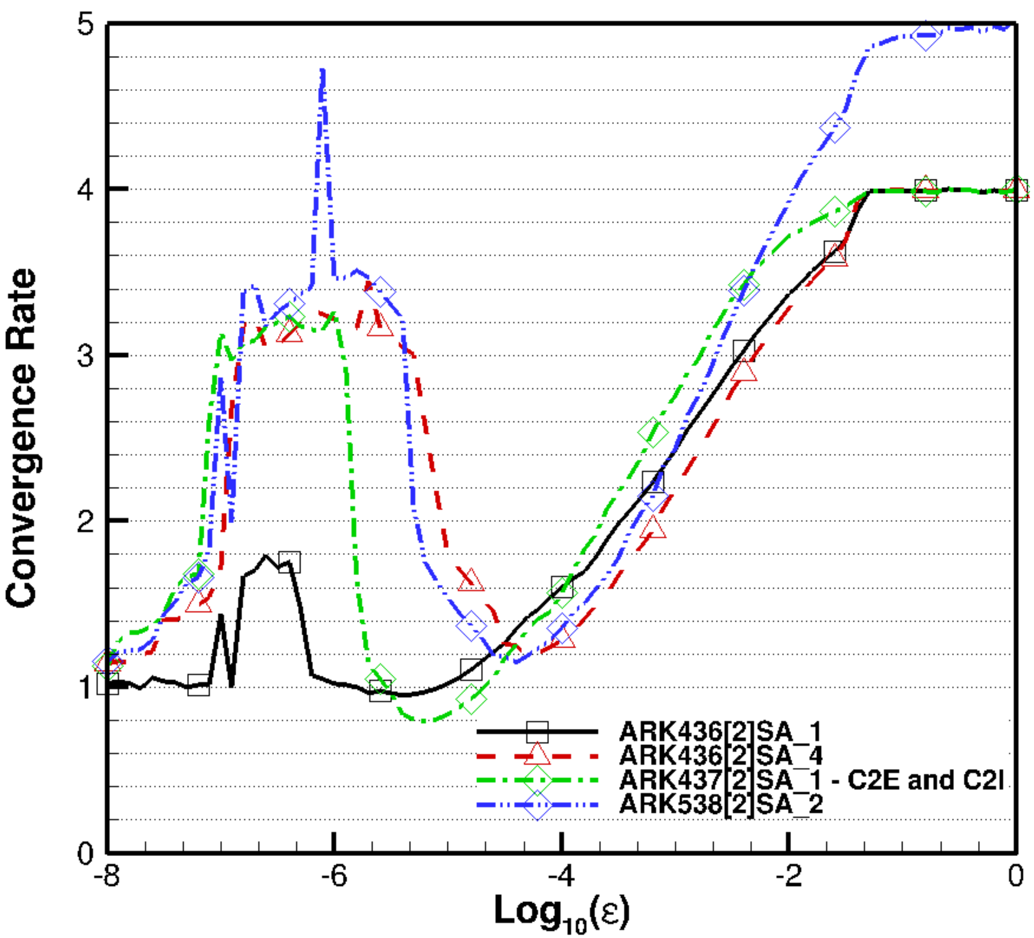
Order Reduction Improvement: Rossler-Chaos

- ARK436[2]SA_1 is baseline scheme
- 5th order ARK538[2]SA_2 and 4th order ARK436[2]SA_4 have similar order reduction
- Multiple schemes on Rossler-Chaos are improvements on baseline



Order Reduction Improvement: Broadwell

- ARK436[2]SA_1 is baseline scheme
- Order reduction improvement is less clear than in other problems



Conclusions

- Built test suite: ~95% idiot proof
- Test suite produces reasonable solutions for each test problem
- Order reduction in new schemes is better than the baseline

- ARK436[2]SA_4 seems to be the best scheme investigated

Future Plans

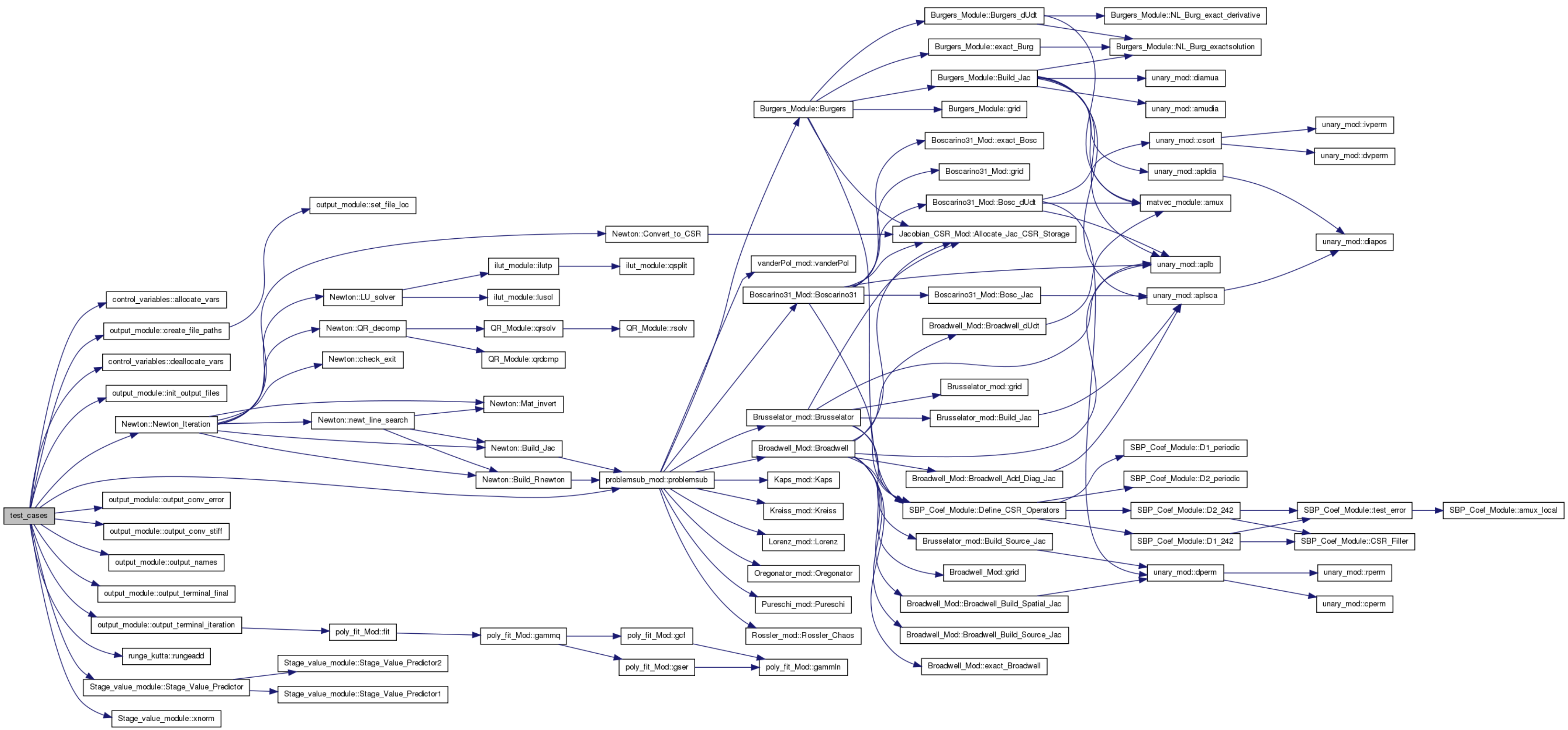
- NASA technical memorandum
  - Long term: journal article
- Implementation into FUN3D

Acknowledgments

- NIFS
- Dr. Mark Carpenter
- Computational AeroSciences Branch

Questions?

Test Suite


test_cases
control_variables::allocate_vars
output_module::create_file_paths
control_variables::deallocate_vars
output_module::init_output_files
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output_module::set_file_loc
Newton::Convert_to_CSR
ilut_module::ilutp
ilut_module::qsplit
Newton::LU_solver
ilut_module::lusol
Newton::QR_decomp
QR_Module::qrsolv
QR_Module::rsolv
Newton::check_exit
QR_Module::qrdcmp
Newton::Mat_invert
Newton::newt_line_search
Newton::Build_Jac
Newton::Build_Rnewton
problemsub_mod::problemsub
output_module::output_conv_error
output_module::output_conv_stiff
output_module::output_names
output_module::output_terminal_final
output_module::output_terminal_iteration
poly_fit_Mod::fit
poly_fit_Mod::gammq
poly_fit_Mod::gcf
poly_fit_Mod::gser
poly_fit_Mod::gammln
runge_kutta::rungeadd
Stage_value_module::Stage_Value_Predictor
Stage_value_module::Stage_Value_Predictor2
Stage_value_module::Stage_Value_Predictor1
Stage_value_module::xnorm
Burgers_Module::Burgers
Burgers_Module::Burgers_dUdt
Burgers_Module::exact_Burg
Burgers_Module::Build_Jac
Burgers_Module::grid
Burgers_Module::NL_Burg_exact_derivative
Burgers_Module::NL_Burg_exactsolution
unary_mod::diamua
unary_mod::amudia
unary_mod::csort
unary_mod::ivperm
unary_mod::dvperm
unary_mod::apldia
matvec_module::amux
unary_mod::diapos
unary_mod::aplb
unary_mod::aplsca
Boscarino31_Mod::exact_Bosc
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Boscarino31_Mod::Bosc_dUdt
Jacobian_CSR_Mod::Allocate_Jac_CSR_Storage
vanderPol_mod::vanderPol
Boscarino31_Mod::Boscarino31
Boscarino31_Mod::Bosc_Jac
Broadwell_Mod::Broadwell_dUdt
Brusselator_mod::grid
Brusselator_mod::Brusselator
Brusselator_mod::Build_Jac
Broadwell_Mod::Broadwell
Broadwell_Mod::Broadwell_Add_Diag_Jac
Kaps_mod::Kaps
Kreiss_mod::Kreiss
Lorenz_mod::Lorenz
Oregonator_mod::Oregonator
Pureschi_mod::Pureschi
Rossler_mod::Rossler_Chaos
SBP_Coef_Module::D1_periodic
SBP_Coef_Module::D2_periodic
SBP_Coef_Module::Define_CSR_Operators
SBP_Coef_Module::D2_242
SBP_Coef_Module::test_error
SBP_Coef_Module::amux_local
SBP_Coef_Module::D1_242
SBP_Coef_Module::CSR_Filler
Brusselator_mod::Build_Source_Jac
Broadwell_Mod::grid
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Broadwell_Mod::Broadwell_Build_Spatial_Jac
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