Automatic Error Estimation and Verification Using an Adaptive Wavelet Method

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11th World Congress on Computational Mechanics (WCCM XI)

Barcelona, Spain, 21 July 2014

Supported by NNSA under the PSAAP II

C-SWARM
Center for Shock Wave-processing of Advanced Reactive Materials

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Motivation

- The Wavelet Adaptive Multilevel Representation (WAMR) enables systems of partial differential equations to be solved to a user-defined error tolerance.
- For many problems, especially those with a few regions of steep gradients, the WAMR method can achieve a solution under a given error threshold with less computational effort than traditional finite difference or finite element methods.
- In contrast to traditional finite difference or finite element methods, WAMR is intrinsically verified.
- We *verify the verification* based on *error tolerance refinement* instead of grid refinement and exercise it on standard challenging test problems in non-linear wave dynamics (Sod, Shu-Osher, etc.).

Verification and Validation

- **Verification**: solving the math right.
- **Validation**: solving the right math.
- Verification is confined to mathematical questions generally involving the comparison of a finite precision prediction against a high precision or exact solution; it is the subject of this presentation.
- Validation speaks to comparison of predictions to experimental data; it will not be considered here.
- We will consider problems with no exact solution and so obtain verification by comparing solutions at a given error tolerance against those with an extremely small error tolerance.

Roache, "Building PDE codes to be verifiable and validatable." *Computing in Science & Engineering* 6(5): 30-38, 2004.

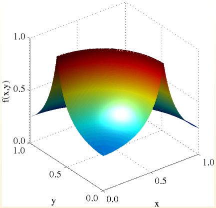
WAMR Method

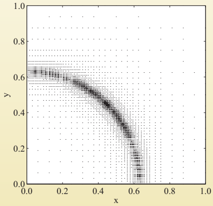
- Represents field variables by projecting them onto a multiscale basis of wavelets.
- Adaptive grid algorithm refines the grid only where it is necessary to meet the user-prescribed error tolerance.
- Collocation points with wavelet amplitudes below the error threshold are removed.
- Similar to wavelet-based JPEG-2000 image compression, the WAMR method compresses the PDE solutions.

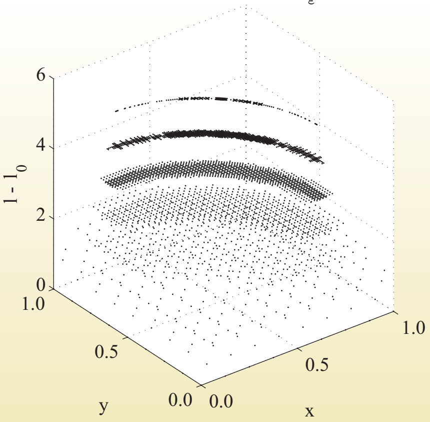
Paolucci, Zikoski, and Wiraseat, "WAMR: An adaptive method for the simulation of compressible reacting flow. Part I. Accuracy and efficiency of algorithm," *J. Comp. Phys.*, 272(1): 814-841, 2014.

Given the threshold parameter ε, the approximation of $u(\mathbf{x})$ becomes

$$u^J(\mathbf{x}) = \underbrace{\sum_{\mathbf{k}} u_{0,\mathbf{k}}\Phi_{0,\mathbf{k}}(\mathbf{x}) + \sum_{j=0}^{J-1} \sum_{\{\boldsymbol{\lambda}\,:\,|d_{j,\boldsymbol{\lambda}}|\geq\varepsilon\}} d_{j,\boldsymbol{\lambda}}\Psi_{j,\boldsymbol{\lambda}}(\mathbf{x})}_{u^J_\varepsilon} + \underbrace{\sum_{j=0}^{J-1} \sum_{\{\boldsymbol{\lambda}\,:\,|d_{j,\boldsymbol{\lambda}}|<\varepsilon\}} d_{j,\boldsymbol{\lambda}}\Psi_{j,\boldsymbol{\lambda}}(\mathbf{x})}_{R^J_\varepsilon},$$







Error in WAMR

- The user-defined error threshold parameter is ϵ.
- The error in the sparse wavelet representation is

$$||U - U_\epsilon^J||_\infty \leq C_1 \epsilon.$$

- The number of collocation points to achieve the error tolerance is

$$N_E \leq C_2 \epsilon^{-d/p}.$$

- The error of a derivative approximation is

$$\left\| \frac{\partial^i U}{\partial x^i} - D_x^{(i)} U_\epsilon^J \right\|_{\boldsymbol{\nu},\infty} \leq C N_E^{-\min((p-i),n)/2}.$$

Navier-Stokes Model for Verification Test Problems

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0,$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\left(\rho u^2 + p - \frac{4}{3}\frac{\tau}{Re}\right) = 0,$$

$$\frac{\partial}{\partial t}\left(\rho\left(\frac{e}{\gamma - 1} + \frac{u^2}{2}\right)\right)$$
$$+\frac{\partial}{\partial x}\left(\rho u\left(\frac{e}{\gamma - 1} + \frac{u^2}{2}\right) + \left(p - \frac{4}{3}\frac{\tau}{Re}\right)u + \frac{\gamma}{\gamma - 1}\frac{q}{RePr}\right) = 0,$$

$$\tau = \frac{\partial u}{\partial x}, \qquad q = -\frac{\partial T}{\partial x}, \qquad p = \rho T, \qquad e = T.$$

$$Re = \frac{\rho_0 a_0 L}{\mu} = 6.526 \times 10^5, \quad Pr = \frac{\mu c_p}{k} = 1.392.$$

Physical diffusion has been added to the test problems to prevent our adaptive method from refining to zero.

Error Evaluation

- A diffusion-based time step is selected so that temporal error smaller than spatial error.
- The error is computed by comparing to a very fine uniform grid solution.
- The error is evaluated for a specific variable at a specific time for all points in the grid.
- The maximum error at a specific time was compared with the prescribed error to verify the predictions.
- Each problem was run for multiple different error thresholds to verify the method for any error threshold with

$$E_U = \left\| \frac{U_n - U_a}{U_a} \right\|_\infty .$$

EVTS Verification Test Problems

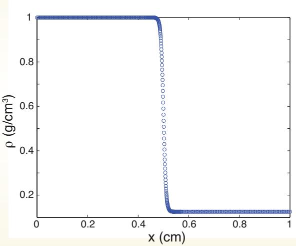
- Three problems were chosen from the Enhanced Verification Test Suite for Physics Simulation Codes (EVTS)
  1. Sod problem,
  2. Modified Sod problem,
  3. Shu-Osher problem,
- They are hydrodynamic shock problems commonly used for code verification.
- Physical viscosity was added as the WAMR requires continuity.
- Our solutions thus incorporate physical diffusion processes ignored in the EVTS problems.

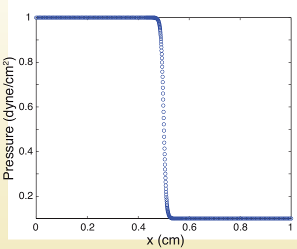
Kamm, et al. "Enhanced verification test suite for physics simulation codes," Los Alamos National Laboratory, LA-14379, 2008.

Sod Problem Initial Conditions

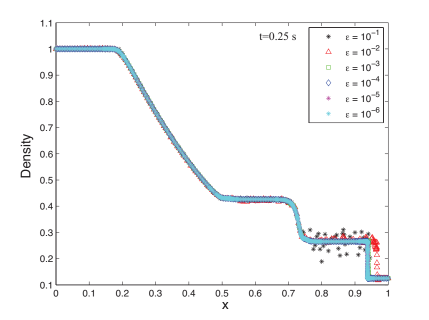
- Models a shock tube filled with N_2 at two different states.
- Diffusion coefficients were assumed to be the values for N_2 at 300 K.
- Initial shock was modeled as tanh.
- EVTS is dimensional; we scaled equations to easier quantify the relative effects of added diffusion.
- EVTS initial conditions are non-physical!

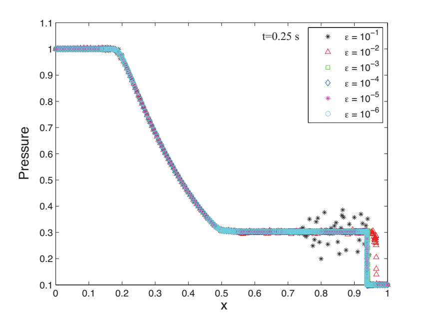
	ρ [g/cm^3]	u [cm/s]	p [dyne/cm^2]
Left	1.0	0.0	1.0
Right	0.125	0.0	0.1
$0 \leq x \leq 1$ cm; $x_i = 0.5$ cm; $t_f = 0.25$ s			



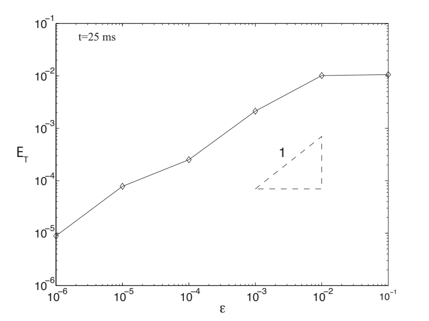


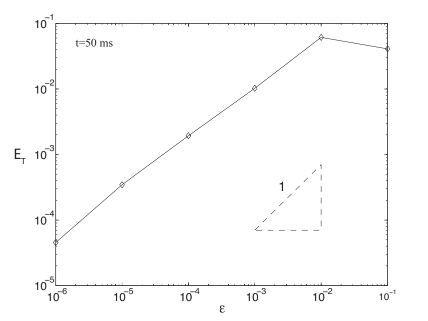
Sod Shock Tube Solutions as Error Tolerance Varies





Error

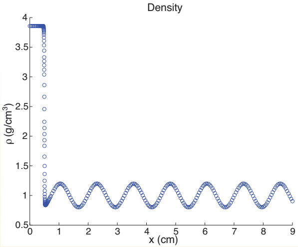


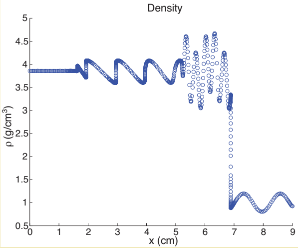


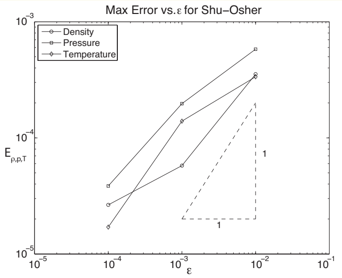
- The achieved error is well predicted by the specified error for a wide range of errors.
- The achieved error grows slowly with time due to integration error.

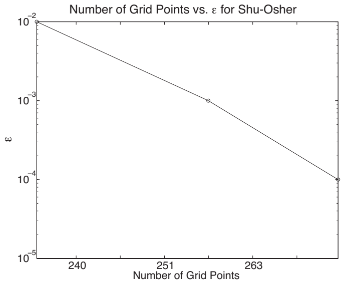
Shu-Osher Problem

	ρ [g/cm^3]	u [cm/s]	p [dyne/cm^2]
Left	3.857143	2.629	10.333
Right	$1+0.2\sin(5x)$	0.0	1.0
$0 \le x \le 9$ cm; $x_i = 4.5$ cm; $t_f = 1.8$ s			



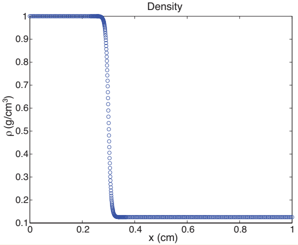


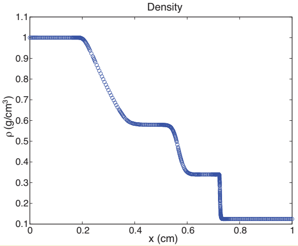


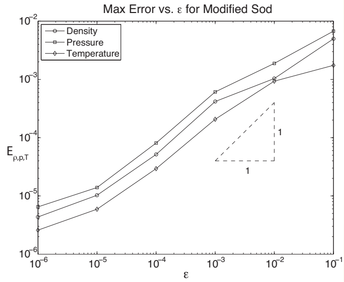


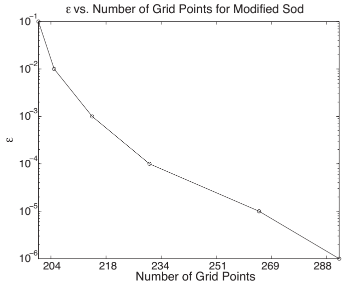
Modified Sod Problem

	ρ [g/cm^3]	u [cm/s]	p [dyne/cm^2]
Left	1.0	0.75	1.0
Right	0.125	0.0	0.1
$0 \le x \le 1$ cm; $x_i = 0.3$ cm; $t_f = 0.2$ s			









Conclusions

- The WAMR method provides automatically verified results based on the user-prescribed error criteria.
- Traditional verification notions such as order of convergence are less relevant for this adaptive method.
- The WAMR method effectively captures the intricacies of advanced hydrodynamic problems
- The adaptive nature of the WAMR method allows one to compute a solution to a specified error in less computational time than competing non-adaptive methods.