# FINAL REPORT

## STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS APPLIED TO THE PREDICTABILITY OF COMPLEX MULTISCALE PHENOMENA



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## DISCLAIMER

# Contents

# A Abstract

The objectives of this research remain as stated in our proposal of November 1997. We report on progress in the quantification of uncertainty and prediction, with applications to flow in porous media and to shock wave physics.

The main strength of this work is an innovative theory for the quantification of uncertainty based on models for solution errors in numerical simulations. We also emphasize a deep connection to application communities, including those in DOE laboratories.

# B Uncertainty Quantification

DOE laboratory collaborators for this work include Merri Wood, Peter Adams, and David Sharp.

The goal includes, but goes beyond error bars for simulations. The goal is to assess the entire scientific environment: data, theory, equations, physics parameters, and simulation, and to arrive at predictions for possible outcomes, with an associated likelihood based on scientific reasoning [17, 18]. Included in this objective are problems such as climate forecasting, for which the deterministic answer many not be unique. That is, the answer many be a probability distribution of possible outcomes.

This program, which was developed within this project and was discussed in previous progress reports, has now been applied to problems within the LANL DP programs, using separate funding [1].

We consider the context of prediction of petroleum production from an oil reservoir. This problem is well known not to have well defined deterministic predictions, due to incomplete information. We also consider uncertainty quantification for shock physics problems. Uncertainty quantification complements and completes the code validation process, as it pertains to the entire science package associated with the code, including physics models, data and parameters as well as numerical and physics approximations in the solution. It offers not just error bars for simulation results, but probabilistic confidence intervals in cases that deterministic bounds are not feasible in view of insufficient information. The general framework, outlined below, applies to both situations as well as to many others.

There are three components to our approach to uncertainty quantification.

- Scale up to achieve rapid simulation of many coarsely gridded problems
- Error analysis to estimate solution error
- Bayesian analysis to compare simulation to data and to arrive at a prediction with quantified uncertainty.

# C Scaleup Models and Methods

## C.1 Scaleup for Petroleum Reservoirs

DOE laboratory collaborators for this work include: David Sharp, Shuling Hou, and Tim Wallstrom.

Our main results are in the stochastic analysis relating up scaled, or averaged, flow to the statistically-described small length-scale fluctuations in the geology. For these nonlinear flow problems, a renormalization group approach to the fractional flow functions and relative permeabilities is required. We follow the scaleup approach of our collaborators [19]. The stochastic aspects of scaleup were studied in Ref. [15]. Scaleup modifies the hyperbolic aspects of the problem (the saturation-dependent wave speeds). Depending on the degree of heterogeneity of the reservoir, the upscaled equations are either deterministic, but different from the primitive ones, or they are random, but with a decreased degree of randomness relative to the primitive equations.

## C.2 Averaged Equations for Multiphase Flow

Our DOE collaborators for this task include: David Sharp, Baolian Cheng, and John Grove.

Chaotic fluid mixing is a major challenge to computational science. We study turbulent fluid mixing layers that form in the late stages of acceleration-driven hydrodynamic instabilities, such as the Rayleigh-Taylor (RT) and Richtmyer-Meshkov (RM) interface instabilities. These instabilities play a central role in laser implosion of inertial confinement fusion targets. The statistical properties of these flows are of primary interest, since the mixing layers are chaotic, with sensitive dependence on initial data.

Our work has the following elements:

- new averaged equations
- models for the motion of the edges of the mixing zone
- DNS simulations, in agreement with experiment, for validation of the averaged equations

We have developed a model [16, 2] of averaged multiphase flow equations which avoids well known pitfalls for multiphase equations. These equations are well-posed mathematically,

free from physical assumptions concerning underdetermined thermodynamical equilibration processes associated with chunk mixed material thermodynamics. The equations have an analytic solution, in closed form, for one-dimensional incompressible flow.

We developed a zero parameter prediction model, in full agreement with all experimental data and theoretical constraints, for the motion of the edges of the mixing zone. The model is a buoyancy drag ODE, and is the first these ODEs to have complete agreement with data. Edge motion models are the main input into our multiphase flow equations [4]. The experimental data contains four independent quantities, namely the growth rate constants for the light and heavy fluid edges (bubbles and spikes) for both RT and RM instabilities. An ODE based on buoyancy and drag has one undetermined parameter, a drag coefficient, for each edge of the mixing zone (*i.e.* a bubble drag coefficient and a spike drag coefficient). The drag coefficient (with its density or Atwood number dependence) is determined from the RT solution of the edge motion. In [5], we give a theoretical calculation of the RT bubble mixing rate, in agreement with experimenal data, through a Renormalization Group bubble merger model. This calculation determines the bubble drag coefficient in the ODE. A principle of nearly constant Center of Mass (COM) for the RT mixing process establishes a link between the RT bubble and spike growth rates [3], thereby giving the RT spike mixing rate and the spike drag coefficient. With the drag coefficients thus parameterized, the ODE is sufficient to determine the RM mixing zone growth constants, in agreement with experiment. The buoyancy drag ODE is solved in closed form for Rayleigh-Taylor and Richtmyer-Meshkov mixing [6]. In the latter case, dependence on initial amipltude is explicit in the leading order asymptotics of the solution.

We study the microphysics through direct numerical simulation (DNS). These simulations will allow validation of the multiphase flow models, such as the one described above. We have a definitive success in DNS simulations of acceleration driven fluid instabilities in agreement with experiment. These simulations used our Front Tracking code FronTier. We also conducted similar simulations using an untracked level set code, and duplicated the results of other groups who found a mixing rate for late time 3D RT simulations below the range of experimental uncertainty [2, 9]. Through this comparison of algorithms [9], we have identified numerical dissipation of interfacial vorticity and density differences (viscosity and mass diffusion) as the principal differences between these algorithms and the presumed cause of the low growth rates.

We have completed an axi-symmetric capability for FronTier. Promising results for axisymmetric simulations have been obtained [11, 10]. These studies will be the basis of a continued study of chaotic mixing in a spherical geometry.

# D Error Models for Scale Up and for Numerical Simulation

## D.1 Error Analysis for Oil Reservoir Simulation

Our DOE collaborators for this task include: David Sharp, Shuling Hou, and Tim Wallstrom.

We developed probabilistic error models to predict the accuracy of scaled up solutions of flow in petroleum reservoirs [13, 12, 14]. The basic method is a nonparametric error model defined by a simulation study of numerical and modeling errors associated with the use of a coarse, or under resolved grid. The error

$$e_j(t) = f_j(t) - c_j(t)$$

is the difference between a fine (regarded as exact) and coarse grid solution for a stochastically determined realization, indexed by $j$. Let $\overline{e} = (1/N)\sum e_j$ be the mean error. We assume that the oil to water production ratio (the oil cut) at the producing well is the primary production observable; the well pressures are also possible observables used in history matching. Thus the $e_j$, $f_j$ and $c_j$ are all oil to water production fractions, as a function of time $t$. The sample error covariance

$$C^s(t_1, t_2) = \frac{1}{N-1}\sum_{j=1}^{N}(e_j(t_1) - \overline{e}_j(t_1))(e_j(t_2) - \overline{e}(t_2))$$

defines a Gaussian measure on observable outcomes of the simulation. The purpose of the solution error model is to define a meaningful measure of the accuracy to be used in the fit to data in a search for possible correct geologies.

A data based study of solution errors must include a more accurate solution as well as the solution of primary interest. For this reason, such studies will be expensive, and cannot be conducted routinely in realistic situations. Thus we assume that the data used to define the error model is itself limited. The statistical consequences of this fact were explored. First a projection onto a finite dimensional space reduces the complexity of the error model to a level consistent with the data. The choice of this dimension and the advantage of smoothing

the data were investigated. Moreover, the covariance used to define the Gaussian error model is itself uncertain and the statistics of this choice was explored, through appeal to a suitable Wishart distribution of possible covariance and precision matrices.

Comparison results to maximum likelihood and simpler parametric error models were obtained.

## D.2 Simulation Error Analysis for Shock Physics

Our DOE collaborators for this task include: David Sharp, John Grove, Karen Pao, Barbara DeVolder, and Tim Wallstrom.

We studied an ensemble of one diemsnional shock wave interaction problems. The ensemble was generated from a base case interaction to allow $\pm 10\%$ variation in selected input parameters [8]. In this way we investigated a stochastic version of the Riemann problem. We believe that the stochastic Riemann problem and its higher dimensional analogues, the stochastic shock polars, will be fundamental in the error analysis for general problems in shock physics, just as the deterministic version of the Riemann problem is fundamental for simulation and analysis of (determinsitic) shock wave physics.

Our main conclusion is to identify various functionals as satisfying approximate Gaussian statistics. These solution functionals include experimentally measurable quantities, such as wave location and arrival times and local space time averages of solution variables. Remarkably, the averaging region required for an approximate Gaussian behavior of the statistics was not very large; a few mesh bolcks sufficed. In contrast, purely local quantities, when evaluated within a propagating solution wave, displayed poor statistical properties, a reflection no doubt of the lack of convergence in the $L_\infty$ norm for numerical approximations.

# E Stochastic Prediction

## E.1 Prediction for Reservoir Flow

Our DOE collaborators for this task include: David Sharp, Shuling Hou, and Tim Wallstrom.

We take one fine grid solution $f_{j_0}(s)$, as data, for some time interval $0 \leq s \leq s_0$, defined as the past. With this knowledge, but without knowing the value of $j_0$ or the geology it defines, we predict the future, $f_{j_0}(s)$, for $s_0 \leq s \leq s_1$. So we consider all possible solutions in the ensemble, the $f_j$ or more realistically the affordable $c_j$. We demand agreement (within a

tolerance) with past data and hope for agreement in the future.

Returning to the simulation study based on Darcy's law in a fully 2D reservoir cross section, and with the the coarse grid upscaled solutions $c_j(s)$ only available for a prediction study, we used a Bayesian approach to define a revised probability in the ensemble of reservoirs, *i.e.* the index space of $j$'s. The original probability for the reservoirs is called the prior distribution. The posterior distribution is obtained from it by multiplication by a likelihood which reflects the likelihood of a mis-match or solution error in comparing the trial solution $c_j(s)$ to the data $f_{j_0}(s)$.

We found an ability to improve on the prior distribution predictions of oil production with a reduction of errors by 30%. Considerable attention was paid to the development of a general methodology, which can be used for other prediction problems. One of our main results was the determination of confidence intervals for prediction. We determined the 5%, 95% confidence intervals for prediction of future oil production. These intervals are dependent on the reservoir selected as exact, and are thus a random variable. Mean values of the upper and lower limits as a per cent of the prediction were determined. These limits were determined for the finely gridded simulations (the "exact" numerics and modeling) and for different levels of upscaling. We found surprisingly small degradation of prediction precision with upscaling from a fine $100 \times 100$ grid to upscaled $20 \times 20$ or $10 \times 10$ grids, and somewhat larger loss of precision for a very aggressive upscaling to a $5 \times 5$ grid. We view this study as the most definitive methodology for assessemnt of upscaling which we are aware of. See [13, 12, 14].

We also considered a simplified, analytically solvable, reservoir model. In this context, a large number of solutions were possible, and the statistics could be fully explored. Remarkably, we found a Markov property for the solution $f_j(s)$. Prediction of the future with knowledge of the past was no more accurate than prediction with knowledge of the present only. A manuscript is in preparation [7].

## E.2 Prediction for Shock Physics Problems

Our DOE collaborators for this task include: David Sharp, Peter Adams, Merri Wood, Charles Nakleh,Karen Pao, Barbara DeVolder, and John Grove.

On the basis of our analysis of solution errors [8], we determined that the spread in solution wave width due to solution error is smaller than that due to the ensemble variation,

assuming a ±10% variation in key input parameters in the defining ensemble. This fact will enable useful prediction and Bayesian analysis on the basis of observations. The prediction step will be taken in the future.

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# H Publications Supported by this Grant


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