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A Population of Linear, Second Order, Elliptic Partial Differential Equations on Rectangular Domains. Part I*

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Abstract. We present a population of 56 linear, two-dimensional elliptic partial differential equations (PDEs) suitable for evaluating numerical methods and software. Forty-two of the PDEs are parametrized which allows much larger populations to be made; 189 specific cases are presented here along with solutions (some are only approximate). Many of the PDEs are artificially created so as to exhibit various mathematical behaviors of interest; the others are taken from "real world" problems in various ways. The population has been structured by introducing measures of complexity of the operator, boundary conditions, solution and problem. The PDEs are first presented in mathematical terms along with contour plots of the 189 specific solutions. Machine-readable descriptions are given in Part 2; many of the PDEs involve lengthy expressions and about a dozen involve extensive tabulations of approximate solutions.

CONTENTS

1. Introduction. The motivation for creating this PDE population is for use in the evaluation of numerical methods and PDE software. The need and rationale for a systematic approach to such evaluations is given in Rice [10], Houstis and Rice [8], Crowder, Dembo and Mulvey [2]; it suffices here to say that a properly chosen problem population is an essential ingredient for a sound evaluation of numerical methods and software.

A useful population of PDEs is inevitably very lengthy and this one is no exception as one sees from the last two appendices. Thus in the body of this paper we discuss the sources of the PDEs, how they are described in the appendices and

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how a structure has been created in the population through the use of quantitative (but subjective) measures of features.

It is important that one be able to create relevant subpopulations as one inevitably wants to evaluate methods for particular subclasses of PDEs (e.g., separable, with singularities or with mixed boundary conditions). Experience shows that no one universal method is best for all PDEs (even in this rather restricted context) and one of the important tasks of research is to create and/or identify methods that are especially efficient for particular classes of PDEs. Once one embarks on such a task one sees that this population, which originally might seem large and bulky, is actually rather small for the uses to be made of it. It is only the fact that it can be substantially expanded in various directions through the parametrization that gives one hope that it is adequate for a wide variety of evaluations.

2. Characteristics of the Problems. A source parameter is assigned to each PDE which ranges from 0 (artificial problem) to 100 (actual real world problem). This feature, as the others introduced later, is subjective in nature and the values given must be taken as approximate indications of our intuitive feelings. The PDE $u_{xx} + u_{yy} = 1$ might be completely artificial for one person and be the actual applications PDE for another. We have at least tried to be consistent in these values.

2.1. *Sources.* Many problems have been normalized so the maximum value of the solution is 1.0 and almost all have this value between .1 and 100. Many of the domains have been standardized to the unit square, $0 \leq x, y \leq 1$. The sources of the PDEs are:

A. *Problems used in previous studies.* Nine problems are included which were used by Eisenstat and Schultz [3] or Houstis et al. [4] and [5]. Subsets of this populaton have been used by Houstis and Papatheodorou [6] and [7] and Lynch and Rice [9]. Some of these PDEs have had parameters added and all have been normalized so the maximum value of the solution is about 1.0.

B. *Artificial problems.* Many problems have been created just to exhibit various mathematical behaviors of interest (e.g. singularities, oscillations or wave fronts). Such behaviors are important for theory or application (or both) and one needs to have them present in the population in an easily identifiable manner.

C. *Problems adapted from the "real world"*. A persistent difficulty is the desire to have PDEs which represent the "real world" and the necessity to know their true solutions. Among the strategies to adapt real world problems we have used:

(i) choosing explicit functions which model the physical solutions and then determining appropriate boundary conditions and/or right side to make this the true solution;

(ii) using truncated series expansions (of high accuracy) with appropriate small modifications in the boundary conditions or right side;

(iii) solving nonlinear problems approximately, then substituting the tabulated numerical solution into the operator (using quadratic interpolation from a 10 by 10 grid) to obtain a linear problem which is, in turn, solved approximately. In these cases the true solution is not known, but the machine-readable population contains tabulated values of a hopefully accurate numerical solution.

2.2. *Problem Features and Complexity Classifications*. We identify as problem features the *smoothness* and *local variation* of operator, the boundary conditions and the solution. These features are quantified on a one-dimensional scale of 0 to 100 even though there are rather independent properties that can be called smoothness or local variation. These features are measured subjectively from the following descriptions of the scale.

Smoothness. This refers to the mathematical properties of the functions or operators involved. Key points on the scale are

00 = entire functions or constants,

10 = analytic; very well behaved,

30 = very smooth, some higher derivative (5 or so) discontinuity possible,

50 = still smooth, third derivative discontinuity possible,

70 = not rough to the eye, but possibly only 1 continuous derivative,

80 = continuous, functions might be theoretically smooth but rough on a gross scale,

90 = possibly discontinuous, nearly singular functions or operators,

100 = strong singularities like $1/x$ or $1/x^2$.

Local variation. This refers to how much a function changes (relative to its size) in a small part of its domain. These variations might be oscillations, wave fronts, peaks or boundary layers. Key points on the scale are

00 = very smooth, uniform,

10 = mild variation, probably convex, some nonuniformity, e.g. $\sin(2x)$, e^{3x} on [0, 1],

25 = modest variation of oscillation; mild wave front or peak, e.g. $\sin(6x)$, $1/(1 + 100x^4)$ on [0, 1],

40 = considerable peak or oscillation; change of magnitude occurs within 10–15% of domain,

60 = sharp peaks, wave fronts, boundary layers or oscillations; 100% change in magnitude occurs within 5% of domain,

75 = practically a discontinuity in magnitude; continuity observable only with a fine scale examination,

90 = actual discontinuity in magnitude; extreme oscillation, step functions, e.g. $\sin(300x)$ on [0, 1].

The overall problem complexity is represented by the average of the above six feature measures. The problems in this population do not have complexities exceeding 58 (only one exceeds 50), a level which might be interpreted as "rather messy with one or two substantial complications". The problem feature measures are included in the descriptions along with the source parameter.

Appendix 1 presents some summary information about the population. Tables are given which

A. group the PDEs according to types of the operator and boundary conditions (e.g. Helmholtz and Dirichlet or constant coefficients and mixed),

B. list the 56 PDEs with abbreviated feature descriptions,

C. group the PDEs according to the smoothness of the operator and right side,

D. group the PDEs according to the smoothness of the solution.

3. Format of Problem Descriptions. Appendix 2 contains a mathematical description of each PDE along with contour plots for each specific instance included in the set of 189 PDEs. An example is shown in Figure 1. The description begins with a problem number and source followed by a mathematical description of the PDE. Then brief comments are given for the operator, right side, boundary conditions, solution and parameters (if any). Sometimes functions appearing in the mathematical description are defined in these comments.

Four generic functions are used:

$f(x, y)$ = right side of PDE determined so that the given true solution is correct.

$f(x)$, $g(y)$ = right sides of boundary conditions determined so that the given true solution is correct.

$T(x, y)$ = the true solution, used in the coefficients of some PDEs derived from nonlinear problems.

$r(x, y)$ = an approximate solution used in some PDEs whose true solution is unknown.

Contour plots are given for one or more particular PDEs for each problem. The border of the plots contains the following information:

(i) values of the parameters, the variables A, B, C, etc. denote α, β, γ, etc.

(ii) maximum and minimum values of the solution; the contours are equispaced between these values.

(iii) the classification parameters in the form

S.P O1.O2 B1.B2 S1.S2

where

S = source parameter	P = problem complexity
$\alpha 1$ = smoothness feature	$\alpha 2$ = local variation feature
and α = O for the operator,	B for the boundary conditions,
	S for the solution.

The machine-readable description of the PDE population consists of two files: EQNFIL and MACFIL. EQNFIL has 189 entries which are either complete statements of the PDE in the ELLPACK language (see Boisvert, Houstis and Rice [1]) or a reference to an entry in MACFIL with values given for parameters. See Figure 2 for a short example. The information given starts with the problem number, feature parameter values and a code for various attributes of the PDE which are used within the ELLPACK system. The machine-readable description uses A, B, C, etc. for α, β, γ, etc. Then ELLPACK language code is given for the operator and boundary conditions; this code should be self explanatory once one sees the UXX$ represents u_{xx}, etc. Finally, there is a Fortran code for any functions that appear in the operator, right side or boundary conditions. This latter code averages about 20 lines and can be as much as 150 lines (excluding tables that are part of some problems). These descriptions are given in Part 2 of this report.

MACFIL entries are just like EQNFIL descriptions of a PDE except that the places where parameter values are to be substituted are indicated by &A, &B, etc. A refers to the first parameter, B the second and so on. There are somewhat more than 8500 lines in these two files.

PROB 28 Artificial

$(wu_x)_x + (wu_y)_y = 1$ where $w = \alpha$ if $0 \le x,y \le 1.$
$\qquad\qquad\qquad\qquad\qquad\quad = 1$ otherwise

DOMAIN $[-1,1] \times [-1,1]$

BC $u = 0$

TRUE unknown

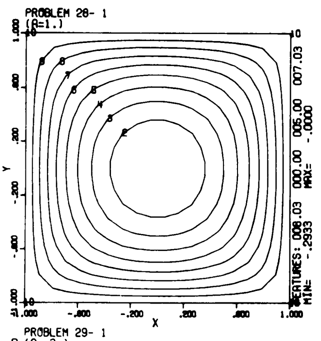
Operator: Self-adjoint, discontinuous coefficients.

Right side: Constant

Boundary conditions: Dirichlet, homogeneous

Solution: Approximate solutions given for $\alpha = 1, 10, 100$. Strong wave fronts for $\alpha \gg 1$.

Parameter: α adjusts size of discontinuity in operator coefficients which introduces large, sharp jumps in solution.



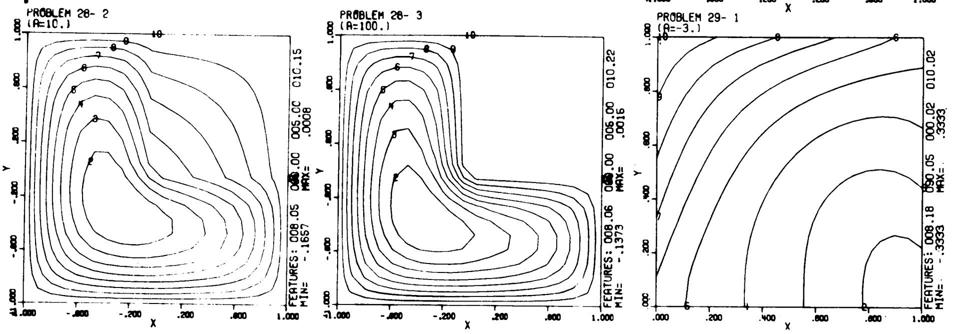


FIGURE 1

An example of the mathematical description of a PDE along with some contours

```
--------------------------------------------------------------------------
'EOR
'EOF
***************
* PROBLEM   2 *
***************
'EOR
*
*          000.04    000.00     004.05     010.02
*          2000200000020
1          TWO DIMENSIONS
1          UXX$ + (1.+Y*Y)UYY$ - UX$ - (1.+Y*Y)UY$ = F(X,Y)
2          MIXED
2          X=0. , MIXED = (1.)U + ( 1.)UX  =  0.27*EXP(Y)
2          X=1. , MIXED = (1.)U + (-1.)UX  =  0.
2          Y=0. , MIXED = (1.)U + ( 1.)UY  =  0.27*EXP(X)
2          Y=1. , MIXED = (1.)U + (-1.)UY  =  0.135*(ALOG(2.)-1.)*(X*X-X)**2
3      FUNCTION TRUE(X,Y)
3      TRUE = 0.135*(EXP(X+Y)+(X*X-X)**2*ALOG(1.+Y*Y))
3      RETURN
3      END
3      FUNCTION F(X,Y)
3      F = 0.135*( (-4.*X*X*X+18.*X*X-14.*X+2.)*ALOG(1.+Y*Y)
3     $     - 2.*((X*X-X)**2)*(Y*Y+Y**3+Y-1.)/(1.+Y*Y) )
3      RETURN
3      END
--------------------------------------------------------------------------
'EOR
'EOF
***************
* PROBLEM   3 *
***************
'EOR
*PARAMETER SET   1(A=1.5)
*          000.43    090.60     000.00     070.40
EXPAND 3/1.5/
'EOR
*PARAMETER SET   2(A=2.5)
*          000.35    080.50     000.00     060.20
EXPAND 3/2.5/
'EOR
*PARAMETER SET   3(A=3.5)
*          000.28    070.30     000.00     050.15
EXPAND 3/3.5/
'EOR
*PARAMETER SET   4(A=4.5)
*          000.23    055.20     000.00     040.20
EXPAND 3/4.5/
--------------------------------------------------------------------------
```

FIGURE 2

A sample from EQNFIL *showing a short PDE description in machine-readable form and a reference to a similar description in* MACFIL

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Appendix 1: Tabulations of Population Characteristics

Table 1

Classifications of Problems According to Operator and Boundary Conditions

Operator	Constant Coefficients			Non-Constant Coefficients		
	Dirichlet	Neumann	Mixed	Dirichlet	Neumann	Mixed
Laplace	3, 4, 7, 8, 10, 11, 17, 33, 34, 35, 47, 50		4, 31, 35, 38, 55			
Helmholtz Type	9, 41, 53			6, 20, 39, 44, 45, 48, 49		
Self-Adjoint	5			1, 13, 22, 25, 28, 54		1, 19, 23, 52
General	14, 46	42	43	12, 15, 16, 18, 21, 26, 27, 29, 30, 32, 36, 37, 56	24	2, 23, 24, 40, 51

Note that problems 1, 4, and 35 appear in two places in the table since they have boundary conditions of the form $u + \alpha u_N = g$ and hence have Dirichlet boundary conditions for $\alpha = 0$. Problem 24 appears in two places since it has boundary conditions of the form $\beta u + u_x + u_y = 0$ and is Neumann for $\beta = 0$.

Table 2

Problem Characteristics

The principal characteristics are tabulated below using the following encodings:

A	Analytic	N	Neumann Boundary Condition
BL	Boundary Layer	NS	Nearly Singular
C	Constant (coefficients)	O	Oscillatory
CC	Computationally Complex	P	Parameterized or Peaked
D	Dirichlet Boundary Condition	S	Singular (infinite)
E	Entire	SD	Singular Derivative
H	Homogeneous	U	Unknown
J	Jump Discontinuity	VS	Variable Smoothness
M	Mixed Boundary Condition	WF	Wave Front

Problem Number	Operator	Right Side	Solution	Boundary Conditions	Domain
1P	A	E	E	M	Unit Square
2	E	A	A	M,H	Unit Square
3P	C	S,SD	S,SD	D,H	Unit Square
4P	C	E	E	M	Unit Square
5P	C	E	E	D,H	Unit Square
6	E,NS	A	A,O	D,H	Unit Square
7	C	C	SD	D,H	Unit Square
8P	C	SD	SD,WF	D	Unit Square
9P	C,NS	E,NS	E,BL	D	Unit Square
10P	C	E,P	E,P	D,H	Unit Square
11P	C	A,O	A,O	D	Unit Square
12P	E,O	E,O	E,O	D	Unit Square
13	J	S	SD	D	Unit Square
14P	C	S	S	D	Unit Square
15P	A,NS	S	SD	D	Unit Square
16P	A,NS	C	U,BL	D,H	Variable Square
17P	C	A,NS	A,NS,WF	D	Unit Square
18P	E	A,NS	A,NS,WF	D	Unit Square
19P	S	S	E	M,H	Square
20P	NS,P,CC	P	E,P	D	Rectangle
21	E	E	E	D	Unit Square
22	SD	S	E	D	Unit Square
23P	SD	SD	SD,WF	M,H	Unit Square
24P	S,NS	S,NS	U,P	M,H	Square
25P	SD	S	E	D,H	Unit Square

Table 2

Problem Characteristics

Problem Number	Operator	Right Side	Solution	Boundary Conditions	Domain
26P	A	A	U, SD	D, H	Variable Square
27	A, NS	C	U, BL	D, H	Square
28P	J	C	U, WF	D, H	Square
29P	S	H	U, VS, BL	D	Unit Square
30P	A, CC	A, CC	A, NS	D	Unit Square
31	C	C	E, (SD)	M	Square
32	A	A	E	D, H	Rectangle
33	C	E	E, O	D	Rectangle
34	C	C	E, (SD)	D	Square
35P	C	H	E, O, BL	M	Square
36P	S	S	A, BL	D	Unit Square
37	E	E	E	D	Unit Square
38P	C	H	E, O, VS	D	Rectangle
39P	CC, S	CC, S	U, BL	D, C	Unit Square
40P	E	A	A	M	Unit Square
41P	C, NS	SD, NS	SD	D, H	Square
42P	C	H	A, O	N	Variable Rectangle
43	C	H	E	M	Square
44P	CC	CC	U, BL	D, H	Unit Square
45P	C, NS	H	U, BL	D	Unit Square
46P	C, NS	H	U, BL	D	Variable Rectangle
47P	C	S	SD, VS	D	Unit Square
48P	CC	CC	U	U	Unit Square
49P	CC	CC	U, SD, BL	D, C	Unit Square
50	C	H	E, O	D	Rectangle
51P	S	C	U, SD, WF	M, H	Unit Square
52P	CC	H	U, O	M, C	Unit Square
53P	C, NS	E, O	E, O	D	Unit Square
54P	E, CC	S, CC	SD, VS	D	Unit Square
55P	C	H	S, VS, BL	M	Rectangle
56P	S	CC	U, O, (SD)	M	Rectangle

Table 3

Classifications of Problems
According to Smoothness of the Operator and Right–Side

(A=Analytic; C=Constants; CC=Computationally Complicated; DD=Discontinuous Derivatives; E=Entire; O=Oscillatory; P=Peak; S=Singular)

Smoothness Operator	Smoothness Right-Side	Problem Numbers
C	C	7, 31, 34, 35, 38, 42, 43, 45, 46, 50, 55
C	E	4, 5, 9, 10. 33, 53
C	A	11, 17
C	DD	3, 8, 41
C	S	3, 14, 47
C	O	6, 11, 53
C	P	10
E	E	12, 21, 37
E	A	2, 6, 18, 40
E	S	54
A	C	16, 27
A	E	1
A	A	26, 30, 32
A	S	15
DD	C	28
DD	DD	13, 23, 25
DD	S	22, 25
S	C	29, 51, 56
S	S	19, 24, 36
O	A	6
O	O	12
C	CC	17, 18
S	CC	56
CC	C	52
CC	P	20
CC	CC	30, 39, 44, 48, 49, 54

Table 4

Classifications of Problems
According to Smoothness of the Solution

Solution Smoothness	Problem Numbers
Entire	1, 4, 5, 9, 10, 12, 19, 20, 21, 22, 25, 31, 32, 33, 34, 35, 37, 38, 43, 50, 53
Analytic	2, 6, 11, 17, 18, 30, 36, 40, 42
Singular Derivatives	3, 7, 13, 14, 15, 41, 47, 51, 54, 56
Oscillatory	6, 11, 12, 33, 35, 38, 42, 50, 53, 56
Wave Front	8, 17, 18, 23, 28, 51
Discontinuous Derivatives	8, 23
Singular	54, 55
Boundary Layer	7, 9, 15, 16, 27, 29, 44, 45, 46, 49
Peak	10, 20, 24
Tabled Solution	16, 24, 26, 27, 28, 29, 39, 44, 45, 46, 48, 49, 51, 52