International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

Nuclear Data Uncertainty Analysis using the coupling of DRAGON with SUSD3D

Adrien Bidaud
Université Joseph Fourier Grenoble, CNRS/IN2P3, Institut National Polytechnique de Grenoble
56 Avenue des Martyrs 38026 Grenoble Cedex, France
bidaud@lpsc.in2p3.fr

Guy Marleau
Institut de génie nucléaire, École Polytechnique de Montréal,
Montréal (QC), Canada
guy.marleau@polymtl.ca

Etienne Noblat
Electricité de France/R&D/ SINETICS,
Clamart, France
etienne.noblat@edf.fr

ABSTRACT

In this paper we present the work performed to make DRAGON [1] (Ecole Polytechnique de Montréal's transport code) and SUSD3D [2] (the nuclear data sensitivity and uncertainty code maintained by OECD) compatible in such a way that extensive nuclear data sensitivities can be evaluated using Generalized Perturbation Theory (GPT) methods [3].
The qualification of this coupling on the Uncertainty Analysis in Modelling (UAM) benchmark is the aim of this paper. We compare the results obtained with this route with TSUNAMI-1D and 3D and with other routes such as the coupling of XSDRNPM to SUSD3D for keff calculations at the cell and assembly levels.
The good consistency between the uncertainty results obtained by very different tools tends to demonstrate that the coupling is effective for keff nuclear data uncertainty calculations. The route proposed here gives uncertainties for criticality that are very comparible with TSUNAMI results.
The capabilities of DRAGON concerning Generalized Adjoint Function open the field for very broad application range of S/U analysis in the future.

Key Words: Uncertainty Analysis, Nuclear Data, Perturbation Theory,

1. INTRODUCTION

GPT Theory has proven to be a very powerful tool for nuclear data sensitivity calculations. In DRAGON, it was first implemented using the collision probabilities formalism [4] and recently generalized to the Methods Of Characteristics [5] (MOC). This will allow the calculation of the adjoint functions associated with linear functional of the flux (such as broad group cross sections and reaction rates) that is required for sensitivity calculations.

OECD NEA distributes a complete set of programs needed for nuclear data uncertainty propagation. ANGELO [6] can be used to check the consistency and to change group structures of covariance matrices. Those matrices can be produced with NJOY (in which the up-to-date ERRORJ module has been recently reintegrated) if the nuclear data uncertainty information is provided in the evaluation file.

SUSD3D folds direct flux, adjoint function, nuclear data and their uncertainties to calculate sensitivities and uncertainties. SUSD3D is able to read angular fluxes or flux moment files coming from various multi-dimensional discrete ordinates codes such as those of DOORS (ANISN, DORT, TORT) and DANTSYS (ONEDANT, TWODANT, THREEDANT and now PARTISN) packages as well as XSDRN (SN 1D solver available in SCALE) and now DRAGON.

The coupling of the two codes will allow the calculation of sensitivity of most of the outputs of neutronics calculation to nuclear data. But it first needs to be qualified against other tools. UAM benchmark provides the perfect framework for this as the route can be compared with a lot of other routes on different exercises representative of classical geometries.

2. WORK DONE TO ALLOW DRAGON AND SUSD3D COUPLING

Coupling DRAGON with SUSD3D implies a reformatting of the DRAGON flux structure to comply with SUSD3D formalism. We chose to give to SUSD3D the binary angular fluxes coming out of Method of cyclic characteristics (MOCC). A specific DRAGON module has been implemented to write flux in DOT XX format that SUSD3D can read. The usual flux moments, consistent with SN formalism, are then computed within SUSD3D.

Classically, deterministic codes calculate and then write angular adjoint functions in reversed order angles and energies. Thus, a particular attention was given for the information concerning the adjoint fonction.

The angular quadrature set (cosinus angles and associated weights) used by DRAGON is written in an ASCII file. DRAGON can produce quadrature set with angles that have a η director cosine equal to zero. This was not expected by SUSD3D as this choice is usually not done by SN codes. This possibility leads to inconsistent reading of the flux by SUSD3D. The solution implemented is to write extremely small value for this cosine so that SUSD3D is forced to read correctly the binary flux file.

Using DRAGON instead of other transport code does not imply any extra work for SUSD3D user anymore.

3 SENSITIVITY VALIDATION

Here we compare the results for cell calculation nuclear data sensitivities obtained by up to five different routes:

1/ the TSUNAMI-1D route which based on XSDRN (1D SN code) direct and adjoint fluxes and TSUNAMI for sensitivity and uncertainty calculation;

2/ the TSUNAMI/SUSD3D which is based on the same SN solutions and SUSD3D as S/U analysis tool;
3/ the TSUNAMI-3D route based on KENO (3D multigroup Monte Carlo) and TSUNAMI as S/U tool;
4/ DRAGON/SUSD3D 69g based on 69 energy group structure MOC calculations of direct and adjoint fluxes and on SUSD3D as S/U tools;
5/ DRAGON/SUSD3D 172g based on 172 energy group structure MOC calculations of direct and adjoint fluxes and on SUSD3D as S/U tools.

When TSUNAMI is used, the implicit term [7] (taking into account for self-shielding effect) is not shown as the other tools are only able to calculate the direct term.

The comparison of sensitivities based on flux coming obtained with very different techniques such as discrete ordinates, methods of characteristics and Monte Carlo could sounds very difficult. Hopefully, the comparison of routes 1 and 2 allows us to separate the S/U tool effects from the effects of the flux solver methodologies. This fact points the importance of the maintenance of different versatile tools by different teams throughout the world to demonstrate tool's qualifications.

3.1. Peach Bottom – Boiling Water Reactor Results

For this exercise we compare all routes. Table I compares the largest energy integrated sensitivities obtained with XSDRN/SUSD3D and DRAGON/SUSD3D with SCALE5/TSUNAMI for a BWR UO2 fuel pin benchmark. The reactions are ordered by their absolute values. Figure 1 presents the comparison of the sensitivities coming from different routes to TSUNAMI-1D one for a better readability of the discrepancies.

Given the qualification of covariance matrices available today, 10% discrepancies between sensitivities are often regarded as good results. For the most important reactions, those appearing on the left hand of Figure 1, sensitivities are very consistent whatever the flux solver or the S/U tool.

For Hydrogen, sensitivities obtained with SUSD3D behave very differently depending on the flux solver overestimating TSUNAMI sensitivities when the same solver is used and underestimating them when they are calculated from DRAGON direct and adjoin functions. Different thermal treatments of H in H2O might explain part of this behavior.

Discrepancies appear to be rather important for elastic or inelastic scattering cross-sections, whatever the nucleus. Sensitivity to scattering cross section is the difference of two terms of high absolute value that are almost equal, making its calculation less forgiving than any other. Even within TSUNAMI the results 1D (based on XSDRN 1D SN code) and 3D (based on Monte Carlo code KENO) results for ^{238}U scattering are not consistent. Thus this trend is not limited to one S/U tool but to the global approach.

The use of different group structure within DRAGON/SUSD3D has almost no impact but for the nucleus with the most important self-shielding factors: capture cross section Uranium 238.

Table I. Peach Bottom-2 BWR unit cell : k_{inf} sensitivities (% k_{inf} / %)

Codes	Tsunami-1d	Xsdrnpm + Susd3d	Dragon + Susd3d		Tsunami-3d
Energy groups	238	238	69	172	238
^{235}U (ν)	9,3459E-01	9,3372E-01	9,2572E-01	9,2585E-01	9,3468E-01
^{235}U (χ)	9,3459E-01	9,3372E-01	9,2572E-01	9,2585E-01	9,3468E-01
^{235}U (n,f)	2,9260E-01	2,9852E-01	3,0519E-01	3,0143E-01	2,9419E-01
^{238}U (n,γ)	-2,6222E-01	-2,5996E-01	-2,9429E-01	-2,5327E-01	-2,6124E-01
^{1}H (n,n)	1,8942E-01	2,2648E-01	6,6591E-02	6,2009E-02	1,8674E-01
^{235}U (n,γ)	-1,3451E-01	-1,3355E-01	-1,3152E-01	-1,3055E-01	-1,3402E-01
^{238}U (ν)	6,5407E-02	6,6284E-02	7,4281E-02	7,4154E-02	6,5323E-02
^{238}U (χ)	6,5407E-02	6,6284E-02	7,4281E-02	7,4154E-02	6,5323E-02
^{1}H (n,γ)	-5,6823E-02	-6,2840E-02	-1,9384E-02	-1,9520E-02	-5,7985E-02
^{238}U (n,f)	3,3321E-02	3,4132E-02	3,9905E-02	3,8020E-02	3,3177E-02
^{238}U (n,n')	-6,1275E-03	-5,8868E-03	-8,2242E-03	-8,6509E-03	-6,2850E-03
^{16}O (n,n)	-5,7780E-03	9,7862E-03	2,3848E-03	-3,5713E-03	-6,2710E-03
^{16}O (n,α)	-4,6303E-03	-4,9304E-03	-3,5923E-03	-3,8573E-03	-4,6137E-03
^{238}U (n,n)	-1,8768E-03	1,0347E-02	2,4891E-04	-1,4029E-03	-3,8442E-03

3.2. TMI-PWR Results

For this exercise, DRAGON was not used. Table II compares the largest energy integrated sensitivities for the PWR UO2 fuel pin benchmark.
This benchmark confirms the trends seen before: no strong discrepancies are observed apart for the reactions implying strong anisotropy such as elastic and inelastic reactions.

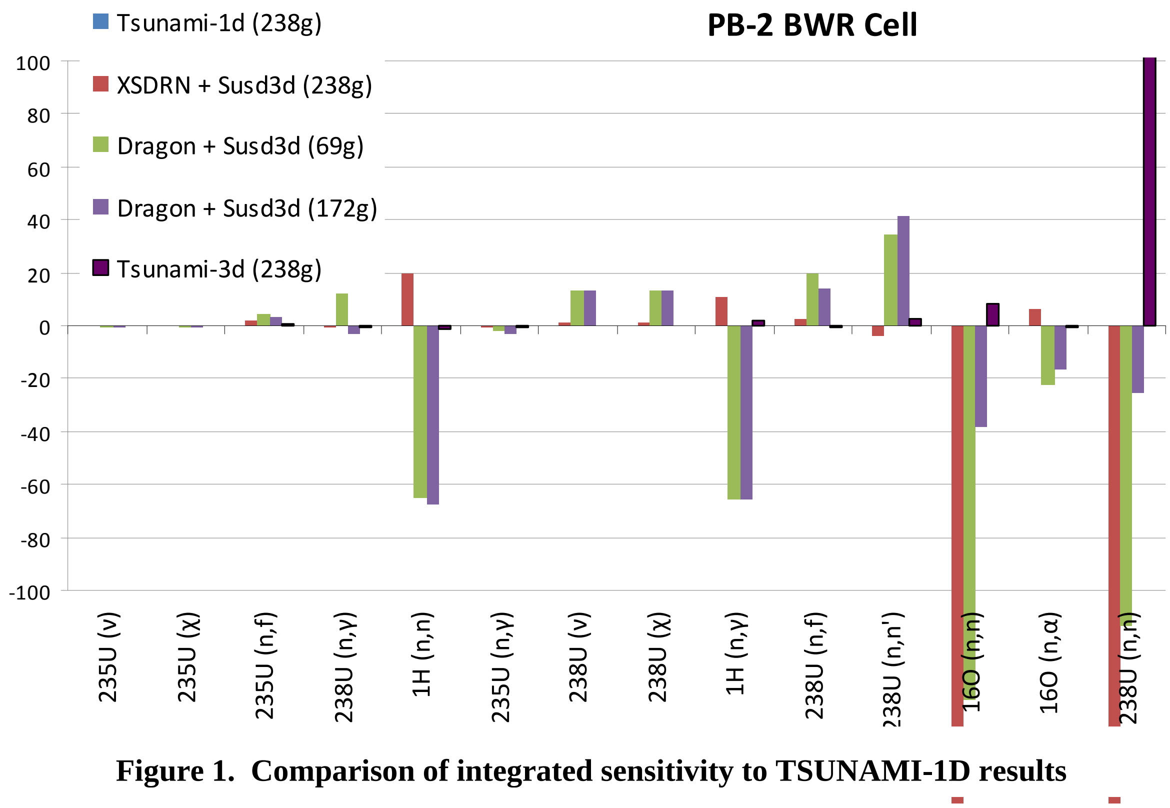

Figure 1. Comparison of integrated sensitivity to TSUNAMI-1D results

Table II. Three Mile Island-1 PWR unit cell : k_{inf} sensitivities (% k_{inf} / %)

Codes	Tsunami-1d	Xsdrnpm + Susd3d	Tsunami-3d
Energy groups	238	238	238
^{235}U (ν)	9,4060E-01	9,3995E-01	9,4037E-01
^{235}U (χ)	9,4060E-01	9,3995E-01	9,4037E-01
^{235}U (n,f)	2,5425E-01	2,6250E-01	2,5290E-01
^{238}U (n,γ)	-2,2286E-01	-2,2027E-01	-2,2299E-01
^{1}H (n,n)	1,8891E-01	2,2191E-01	1,8896E-01
^{235}U (n,γ)	-1,5417E-01	-1,5292E-01	-1,5418E-01
^{238}U (ν)	5,9400E-02	6,0049E-02	5,9634E-02
^{238}U (χ)	5,9400E-02	6,0049E-02	5,9634E-02
^{1}H (n,γ)	-3,7954E-02	-4,1862E-02	-5,9634E-02
^{238}U (n,f)	2,8554E-02	2,9228E-02	3,8785E-02
Zr (n,γ)	-8,3269E-03	-1,0159E-02	-8,3244E-03
^{238}U (n,n')	-5,1866E-03	-4,7949E-03	-5,1027E-03
^{16}O (n,n)	-4,8010E-03	8,8905E-03	-5,2338E-03
^{16}O (n,α)	-4,6490E-03	-4,9421E-03	-4,6164E-03
^{238}U (n,n)	-1,7708E-03	8,8103E-03	-3,5880E-03
Zr (n,n')	-1,5472E-03	-1,6344E-03	-1,3860E-03

3.3. Kozloduy-6-VVER Results

For this exercise, neither DRAGON nor KENA were used. Only the effect of using different S/U analysis tools was tested. Table II compares the largest energy integrated sensitivities for the PWR UO2 fuel pin benchmark.
This benchmark also confirms the trends seen before: no strong discrepancies are observed apart for the reaction implying strong anisotropy such as elastic and inelastic reactions.

Table V. Kozloduy-6 VVER unit cell : k_{inf} sensitivities (% k_{inf} / %)

Codes	Tsunami-1d	Xsdrnpm + Susd3d
Energy groups	**238**	**238**
^{235}U (ν)	9,3888E-01	9,3800E-01
^{235}U (χ)	9,3888E-01	9,3800E-01
^{235}U (n,f)	2,8379E-01	2,8764E-01
^{238}U (n,γ)	-2,6190E-01	-2,5618E-01
^{1}H (n,n)	1,9680E-01	2,3929E-01
^{235}U (n,γ)	-1,3932E-01	-1,3879E-01
^{238}U (ν)	6,1124E-02	6,1996E-02
^{238}U (χ)	6,1124E-02	6,1996E-02
^{1}H (n,γ)	-5,0832E-02	-5,6291E-02
^{238}U (n,f)	3,1135E-02	3,1875E-02
Zr (n,γ)	-1,2172E-02	-1,4890E-02
^{238}U (n,n')	-5,3790E-03	-5,5362E-03
^{16}O (n,n)	-4,9719E-03	4,7139E-03
^{16}O (n,α)	-4,5135E-03	-4,8261E-03
^{238}U (n,n)	-2,1282E-03	4,4000E-03
Zr (n,n')	-2,1089E-03	-2,2345E-03
^{93}Nb (n,γ)	-1,1423E-03	-1,2808E-03

4 UNCERTAINTY VALIDATION

4.1 Origin of the uncertainties.

The uncertainties for cross sections are coming from the 44 groups structure covariance matrices library available in SCALE. The group structure of those matrices was adapted to each case using ANGELO [6].

This procedure was used for all nuclear data but for fission neutron spectrum (**χ**) that is not the same in TSUNAMI and in SUSD3D. For SUSD3D, the data where prepared by NJOY/ERRORR module from the JENDL3.3 library. JENDL estimate of uncertainty on fission neutron spectrum is almost 3 times larger than SCALE's one. The impact is about 100pcm in TSUNAMI and 250pcm in SUSD3D. One should remind that the total uncertainty is the root of the square of each contribution. This means that the uncertainty on χ would almost not contribute to the total if SCALE guess is taken and should not be forgiven if JENDL one is used. The object of this paper is not to discuss the quality of available uncertainty. That is why we don't show it here in the tables. This would add a source of discrepancies that is very large when compared to those coming from differences in the processing of the fluxes or of the sensitivities.

4.2 General discussion

The agreement between the sensitivities is translated to agreement in the uncertainties. All the trends are independent of the benchmark definition. The geometry details have little impact on the contribution of the most important reactions. As far as slightly enriched uranium and light water are used, the contributions of reactions on Uranium isotopes always dominate the uncertainty on keff.

Most uncertainties obtained by various tools but those implying elastic or inelastic scattering are quite consistent. Anisotropy is involved in those reactions. And the treatment of this anisotropy has strong impact on sensitivities and therein on uncertainties. This is the main source of discrepancies among all routes for the total uncertainty that are globally coherent. The discrepancies between sensitivities for ^{238}U elastic scattering are so large that the sign of the contribution of the correlation between scattering and capture cross sections for ^{238}U seems unknown.

Despite the capabilities of SUSD3D to use the uncertainty on double differential cross section (that could be stored in MF 34 in ENDF format), this information is never used.

4.1. Peach Bottom -BWR Results

Table IV compares the largest energy integrated sensitivities for the BWR UO2 fuel pin benchmark.

4.2. Three Mile Island-1 PWR Results

Table V compares the largest energy integrated sensitivities for the BWR UO2 fuel pin benchmark.

Table IV. Peach Bottom-2 BWR unit cell : k_{inf} uncertainty parts (Δkinf / kinf (%))

Codes	Tsunami-1d	Xsdrnpm + Susd3d	Dragon + Susd3d		Tsunami-3d
Energy groups	**238**	**238**	**69**	**172**	**238**
Total	0,5135	0,5395	0,6062	0,5142	0,5459
^{238}U (n,γ)	3,6096E-01	3,8092E-01	4,9564E-01	3,7120E-01	3,7682E-01
^{235}U (ν)	2,7154E-01	2,7124E-01	2,6879E-01	4,5798E-02	2,7184E-01
^{235}U (n,γ)	1,7306E-01	1,7303E-01	1,7336E-01	1,6686E-01	1,7141E-01
^{235}U (n,f)	1,0432E-01	1,0951E-01	1,1558E-01	1,1294E-01	1,0380E-01
^{238}U (n,n) , ^{238}U (n,γ)	-1,0406E-01	3,0235E-02	4,4963E-03	4,0983E-02	1,6010E-01
^{238}U (n,f)	7,5296E-02	5,1566E-02	3,4248E-02	5,1247E-02	7,2166E-02
^{16}O (n,α)	5,2828E-02	5,7031E-02	3,8744E-02	4,4138E-02	5,2821E-02
^{238}U (ν)	3,9837E-02	4,0269E-02	4,6857E-02	4,5798E-02	3,9827E-02
^{1}H (n,n)	3,2581E-02	3,9342E-02	1,1123E-02	1,1184E-02	3,2638E-02
^{238}U (n,n)	2,9577E-02	1,1699E-02	2,1563E-04	9,1630E-03	2,8629E-02
^{1}H (n,γ)	2,8423E-02	3,1433E-02	9,6964E-03	9,7644E-03	2,9006E-02
^{238}U (n,n')	2,4581E-02	2,8066E-02	3,5506E-02	3,7772E-02	2,4291E-02
^{16}O (n,n)	1,3251E-02	1,1749E-02	6,0020E-03	7,8497E-03	1,1350E-02

Table V. Three Mile Island-1 PWR unit cell : k_{inf} uncertainty parts (Δkinf / kinf (%))

Codes	Tsunami-1d	Xsdrnpm + Susd3d	Tsunami-3d
Energy groups	**238**	**238**	**238**
Total	0,4961	0,5182	0,5282
^{238}U (n,γ)	2,9553E-01	3,1569E-01	3,1517E-01
^{235}U (ν)	2,6470E-01	2,6444E-01	2,6474E-01
^{235}U (n,γ)	2,4609E-01	2,4670E-01	2,4563E-01
^{235}U (n,f)	1,2374E-01	1,3327E-01	1,2291E-01
^{238}U (n,n) , ^{238}U (n,γ)	-1,0612E-01	3,5117E-02	1,1021E-01
Zr (n,γ)	7,0617E-02	9,3911E-02	7,0843E-02
^{238}U (n,f)	6,3406E-02	4,2795E-02	6,1169E-02
^{16}O (n,α)	5,3013E-02	5,7131E-02	5,2661E-02
^{238}U (ν)	3,6183E-02	3,6487E-02	3,6327E-02
^{238}U (n,n)	3,2350E-02	1,2676E-02	2,7109E-02
^{1}H (n,n)	3,1146E-02	3,7773E-02	3,1889E-02
^{238}U (n,n')	2,0760E-02	2,3345E-02	1,8078E-02
^{1}H (n,γ)	1,8990E-02	2,0946E-02	1,9406E-02
^{16}O (n,n)	1,1963E-02	1,0262E-02	8,5602E-03
Zr (n,n')	1,1240E-02	1,1864E-02	9,9690E-03

4.3. Kozloduy-6-VVER Results

Table VI compares the largest energy integrated sensitivities for the BWR UO2 fuel pin benchmark.

Table VI. Kozloduy-6 VVER unit cell : k_{inf} uncertainty parts (Δkinf / kinf (%))

Codes	Tsunami-1d	Xsdrnpm + Susd3d
Energy groups	**238**	**238**
Total	0,5142	0,5443
^{238}U (n,γ)	3,6124E-01	3,7892E-01
^{235}U (ν)	2,7155E-01	2,7125E-01
^{235}U (n,γ)	1,8743E-01	1,8793E-01
^{238}U (n,n) , ^{238}U (n,γ)	-1,3033E-01	5,2981E-02
^{235}U (n,f)	1,0669E-01	1,1143E-01
Zr (n,γ)	9,0735E-02	1,2347E-01
^{238}U (n,f)	7,2537E-02	4,7697E-02
^{16}O (n,α)	5,1485E-02	5,5813E-02
^{238}U (n,n)	4,1298E-02	1,7611E-02
^{238}U (ν)	3,7227E-02	3,7663E-02
^{1}H (n,n)	3,2338E-02	4,0213E-02
^{1}H (n,γ)	2,5431E-02	2,8158E-02
^{238}U (n,n')	2,1408E-02	2,5131E-02
Zr (n,n')	1,5376E-02	1,6282E-02
^{16}O (n,n)	1,2880E-02	8,3862E-03
^{93}Nb (n,γ)	1,1010E-02	1,2347E-02

5. CONCLUSIONS

In this paper, extensive comparison of various combinations of codes was done. All the combinations give very comparable results for nuclear data global uncertainty for criticality. The contributions of the most important reactions are remarkably coherent. This means that most of the physics of the propagation of nuclear data uncertainties is reasonably understood for such simple cases and that one can use those tools with confidence if enough precautions are taken.

The smaller contributions of reactions with lower sensitivities or uncertainties do not show so good consistency. In particular, it seems that the estimation of the contribution of reactions concerned with anisotropy is not so well understood. It seems that sensitivities to scattering cross sections will require extra efforts. Eventually, as scattering cross sections have little absolute uncertainties in readily available covariance matrices, the total uncertainties given by different routes shows the same trends : ie uncertainty on keff of about 500pcm (0,5%) dominated by ^{238}U capture cross section and ^{235}U neutron fission yield and capture cross section.

Given the impact of correlations between reaction channels in the final uncertainty evaluation, it seems that these correlations and of the correlation between nucleus should be evaluated with the highest care as possible. Those extra terms would be useful as we have shown that S/U codes are able to handle them and that their impact might not be negligible.

This work shows that the coupling of DRAGON with SUSD3D seems to work very fine. This is very encouraging because of the large field of sensitivities that can be calculated given the Generalized Perturbation capabilities of DRAGON. This is also encouraging from the point of view of the sensitivities as this new tool will be very valuable for S/U code qualification by confirming the trends observed in the results of other flux solvers.

We hope that this work will contribute to motivate the international effort on nuclear data uncertainty evaluation.

ACKNOWLEDGMENTS

This work would not have been done without the support of the group of Nuclear Reactor Physics of the LPSC, of the International Office of PHELMA/INPG and of the Ecole Polytechnique de Montreal. Ivo Kodeli, must be thanked for his numerous piece of advice in the use of SUSD3D.

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