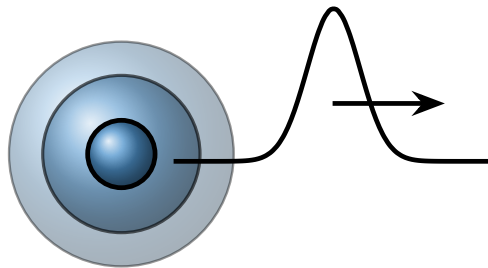

APECSS

(Acoustic Pulse Emitted by Cavitation in Spherical Symmetry)



Fabian Denner
Sören Schenke

24 October 2022

Contents

| | | |
|----------|---------------------------------------|-----------|
| 1 | About APECSS | 3 |
| 2 | Using APECSS | 4 |
| 2.1 | Installation | 4 |
| 2.2 | Running APECSS | 4 |
| 2.2.1 | The *.apecss options file | 4 |
| 2.2.2 | Examples | 5 |
| 2.3 | Units | 5 |
| 2.4 | Programming in APECSS | 5 |
| 2.4.1 | Macros | 6 |
| 2.4.2 | Structures | 8 |
| 2.4.3 | A word on function pointers | 8 |
| 2.4.4 | Code formatting | 9 |
| 2.5 | Important functions | 9 |
| 3 | Bubble dynamics | 11 |
| 3.1 | Rayleigh-Plesset models | 11 |
| 3.2 | The gas | 12 |
| 3.3 | The liquid | 14 |
| 3.3.1 | Equation of state | 15 |
| 3.3.2 | Viscoelasticity | 15 |
| 3.4 | The interface | 17 |
| 3.5 | Infinity | 19 |
| 3.6 | Results | 19 |
| 4 | Acoustic emissions | 21 |
| 4.1 | Lagrangian wave tracking | 21 |
| 4.2 | Incompressible assumption | 22 |

| | | |
|-----|--|----|
| 4.3 | Quasi-acoustic model | 22 |
| 4.4 | Emissions based on the Kirkwood-Bethe hypothesis | 23 |
| 4.5 | Results | 24 |

| | | |
|---------------------|--|-----------|
| Bibliography | | 25 |
|---------------------|--|-----------|

Chapter 1

About APECSS

APECSS is a software tool to compute pressure-driven bubble dynamics and the resulting acoustic emissions. It is written exclusively in C and has been developed with simplicity, versatility and performance in mind. The acronym APECSS stands for "Acoustic Pulse Emitted by Cavitation in Spherical Symmetry".

The main features of APECSS are:

- Bubble dynamics using widely-used models for the bubble dynamics (Rayleigh-Plesset, Keller-Miksis, Gilmore).
- Acoustic emissions of the bubble under different assumptions (incompressible, quasi-acoustic, fully compressible).
- Prediction of the formation and attenuation of shock fronts emitted by the bubble.
- Viscoelastic media (Kelvin-Voigt, Zener, Oldroyd-B).
- Lipid monolayer coating of the bubble as used for ultrasound contrast agents.
- All ODEs are solved with an in-built fifth-order Runge-Kutta scheme with fourth-order error estimate, based on Dormand and Prince [5].
- APECSS has no external dependencies, aside from the standard *math* library and some common C headers (*math.h*, *stdio.h*, *stdlib.h*, *string.h*).

The APECSS repository is located at <https://github.com/polycfd/apecss> and structured as follows:

- The `documentation/` folder contains this short documentation of APECSS.
- The `examples/` folder contains representative examples of how to use APECSS and to demonstrate the most important features of APECSS.
- The `include/` folder contains the `apecss.h` header file, in which all variables, macros and functions of APECSS are defined.
- The `lib/` folder in which the APECSS library is compiled (at least if you follow the installation instructions in Section 2.1).
- The `src/` folder contains all source files (`*.c`) of APECSS.
- The `.clang-format` file, which defines the formatting rules for the source code, see Section 2.4.4.
- The `.gitignore` file telling *git* which folders and files to ignore.
- The `LICENSE.txt` file containing the Mozilla Public License Version 2.0.
- The `README.md` file with the most important information about APECSS.

APECSS is under the copyright of its developers and made available as open-source software under the terms of the [Mozilla Public License Version 2.0](#).

The development of APECSS has directly benefitted from research funding provided by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), grant number 441063377.

Chapter 2

Using APECSS

2.1 Installation

Installing APECSS is easy. After downloading APECSS in the folder `<path to APECSS>`, define the following environment variables:

- `APECSS_DIR` to the folder in which APECSS is located. Using `bash`, for instance, simply execute the command `export APECSS_DIR=<path to APECSS>` or, even better, add this command to your `bash` profile.
- `USRLIB_DIR` to the folder in which `libm.a` or `libm.dylib` (the standard *math* library) is located. This may, for instance, be `/usr/lib64/` on Linux systems or `/usr/lib/` on MacOS systems.

Now, navigate into the folder `$APECSS_DIR/lib` and execute `./compile_lib.sh`. This shell script will compile the APECSS library using `cmake` with the `CMakeLists.txt` file provided in this folder. By default, APECSS is compiled with double precision and in *Release* mode, meaning all optimization flags are enabled. That's it, you've successfully installed APECSS!

2.2 Running APECSS

There are several ways in which you can use the APECSS library. You can either incorporate selected features of APECSS into your own software code or you can program an interface to use APECSS as a standalone program.

2.2.1 The `*.apecss` options file

The `*.apecss` file is the primary way of passing options, such as the size of the bubble, the density of the liquid or the type of results you want to have written out, to APECSS.

Any `*.apecss` file may contain the following sections (each terminated with `END`):

- **BUBBLE**: Information related to the bubble, such as its initial radius R_0 or the Rayleigh-Plesset model that is used to solve its dynamics.
- **GAS**: Properties and equation of state of the gas.
- **LIQUID**: Properties, type (i.e. Newtonian or viscoelastic) and equation of state of the liquid.
- **INTERFACE**: Properties of the gas-liquid interface.
- **RESULTS**: Results of the bubble dynamics and the acoustic emissions that should be written out.
- **ODESOLVER**: Parameters of the ODE solver.

The options file is read by the function `apecss_options_readfile()`. Any of the sections in the `*.apecss` file, and any of the options that may be defined within each section, are optional; they are read if they are present, otherwise the default values (typically set in `apecss_*.setdefaultoptions()`) or values set in the code calling it will be used. Comments can be added using `#`.

The relevant options that are available are discussed in the following chapters of this documentation in the context of the theoretical framework of APECSS. For instance, the available options used to define a certain Rayleigh-Plesset model are discussed in Section 3.1, where the theory of the implemented Rayleigh-Plesset models is described.

2.2.2 Examples

Some representative examples are available in the `$APECSS_DIR/examples` folder. Each directory contains the following:

- A `README.md` file explaining the purpose and specificities of this/these example(s).
- A `src/` folder with a file called `*.apecss.c` that acts as the standalone interface to the APECSS library. This file contains the `main()` function and any additional functionality required to simulate a specific scenario.
- A `build/` folder containing the `CMakeLists.txt` file and a shell script `compile.sh` with which this example can be compiled using the command `./compile.sh`.
- One or several `*.apecss` files in which the options for a specific case are defined.

In the examples provided in the `$APECSS_DIR/examples` folder, the name of the `*.apecss` file is passed as an argument with the call to run APECSS, e.g. executing `./<APECSS-example> -options run.apecss` to use an options file named `run.apecss`.

Detailed information about each example, how to run it and what the results might be compared to can be found in the accompanying `README.md` file.

2.3 Units

APECSS assumes SI units or any appropriate combination of SI units at all times, e.g. when reading user-defined options and in all internal computations. To avoid any misunderstanding, the SI base units are the following:

- Time in seconds [s]
- Length in meter [m]
- Mass in kilogram [kg]
- Temperature in Kelvin [K]
- Electric current in Ampere [A]
- Amount of substance in mole [mol]
- Luminosity in candela [cd]

2.4 Programming in APECSS

All functions are located in source files (`*.c`) that relate to parts of the code, distinguished by physical phenomena (e.g. `emissions.c`), fluid type (e.g. `liquid.c`) or computational operations (e.g. `results.c`).

All declarations and definitions are located in the header file `apecss.h`.

2.4.1 Macros

Macros are used as shortcuts to define frequently-used constants (e.g. `APECSS_PI`), for frequently-used computational operations (e.g. `APECSS_MAX`) and for computational operations that depend on the chosen machine precision (e.g. `APECSS_SQRT`). Furthermore, options related to different numerical models are represented by logically named flags.

2.4.1.1 Macros related to machine precision

APECSS can be used with different floating point precisions: double precision (default) and long double precision (`APECSS_PRECISION_LONGDOUBLE`).

Based on the chosen precision, `APECSS_FLOAT` is defined as the standard floating point type. In addition, the following precision-dependent computational operations are defined based on the chosen floating point precision:

- `APECSS_ABS(a)`: Absolute value of a .
- `APECSS_CEIL(a)`: a rounded to the nearest integer larger than a .
- `APECSS_COS(a)`: Cosine of a .
- `APECSS_EPS`: Returns a value that is close to machine epsilon.
- `APECSS_EXP(a)`: e to the power a .
- `APECSS_LOG(a)`: Natural logarithm of a .
- `APECSS_POW(a,b)`: a to the power b .
- `APECSS_SIN(a)`: Sine of a .
- `APECSS_SMALL`: Returns a number significantly smaller than machine epsilon.
- `APECSS_SQRT(a)`: Square root of a .
- `APECSS_STRINGTOFLOAT(a)`: Conversion of string a to a float.

To ensure compatibility for different floating point precisions, it is paramount to use the standard floating point type `APECSS_FLOAT` and the operator definitions given above consistently throughout APECSS.

2.4.1.2 Computational operations and predefined constants

Macros that provide a shortcut to frequently-used computational operations are:

- `APECSS_POW2(a)`: Returns a^2 .
- `APECSS_POW3(a)`: Returns a^3 .
- `APECSS_POW4(a)`: Returns a^4 .
- `APECSS_MAX(a,b)`: Returns the maximum of a and b .
- `APECSS_MAX3(a,b,c)`: Returns the maximum of a , b and c .
- `APECSS_MIN(a,b)`: Returns the minimum of a and b .
- `APECSS_MIN3(a,b,c)`: Returns the minimum of a , b and c .

Macros that provide a shortcut to frequently-used constants are:

- `APECSS_PI`: Returns π .
- `APECSS_E`: Returns e .
- `APECSS_ONETHIRD`: Returns $1/3$.
- `APECSS_ONESIXTH`: Returns $1/6$.
- `APECSS_AVOGADRO`: Returns the Avogadro constant.
- `APECSS_LN_OF_2`: Returns the natural logarithm of 2.
- `APECSS_LN_OF_10`: Returns the natural logarithm of 10.
- `APECSS_LARGE`: Returns a large number, defined as 10^{15} .

2.4.1.3 Flags for model options

All model options are represented by human-readable flags.

If explicitly indicated as such, these flags are defined in such a way (with integer values being a multiple of 2), that a bit-wise comparison can be performed. Bit-wise comparison may be used for options that are checked frequently and for options that can have several building blocks.

Options of the Runge-Kutta scheme used to discretize the ODEs:

- APECSS_RK54_7M: RK5(4)7M (minimum truncation) coefficients of Dormand and Prince [5]
- APECSS_RK54_7S: RK5(4)7S (stability optimized) coefficients of Dormand and Prince [5]

Rayleigh-Plesset schemes:

- APECSS_BUBBLEMODEL_RP: Standard Rayleigh-Plesset model, Eq. (3.1).
- APECSS_BUBBLEMODEL_RP_ACOUSTICRADIATION: Rayleigh-Plesset model with acoustic radiation damping, Eq. (3.2).
- APECSS_BUBBLEMODEL_KELLERMIKSIS: Keller-Miksis model, Eq. (3.3).
- APECSS_BUBBLEMODEL_GILMORE: Gilmore model, Eq. (3.4).

Equation of state of the gas:

- APECSS_GAS_IG: Ideal gas EoS.
- APECSS_GAS_HC: Ideal gas EoS with van-der-Waals hardcore.
- APECSS_GAS_NASG: Noble-Abel-stiffened-gas EoS.

Equation of state of the liquid:

- APECSS_LIQUID_TAIT: Tait EoS.
- APECSS_LIQUID_NASG: Noble-Abel-stiffened-gas EoS.

Viscoelasticity of the liquid:

- APECSS_LIQUID_NEWTONIAN: Newtonian liquid.
- APECSS_LIQUID_KELVINVOIGT: Kelvin-Voigt solid.
- APECSS_LIQUID_ZENER: Zener solid (standard linear solid model).
- APECSS_LIQUID_OLDROYDB: Oldroyd-B liquid.

Lipid monolayer coating of the gas-liquid interface (bit-wise):

- APECSS_LIPIDCOATING_NONE: No lipid monolayer coating.
- APECSS_LIPIDCOATING_MARMOTTANT: Lipid monolayer coating described by the model of Marmottant *et al.* [16].
- APECSS_LIPIDCOATING_GOMPERTZFUNCTION: Redefine the Marmottant model with a Gompertz function [8].

Acoustic excitation applied to the bubble:

- APECSS_EXCITATION_NONE: No external excitation.
- APECSS_EXCITATION_SIN: Sinusoidal excitation.

Model to compute the acoustic emissions of the bubble:

- APECSS_EMISSION_NONE: Emissions are not modelled.
- APECSS_EMISSION_INCOMPRESSIBLE: Emissions are assumed to occur in an incompressible fluid.
- APECSS_EMISSION_FINITE_TIME_INCOMPRESSIBLE: Emissions are assumed to occur in an incompressible fluid, but the finite propagation speed given by the speed of sound is taken into account.
- APECSS_EMISSION_QUASIACOUSTIC: Emissions are modelled under the quasi-acoustic assumption of Gilmore [7].
- APECSS_EMISSION_KIRKWOODBETHE: Emissions are modelled based on the Kirkwood-Bethe hypothesis.

2.4.1.4 Others

Other predefined macros are used to define the length of strings and arrays, as well as to help with debugging:

- `APECSS_DATA_ALLOC_INCREMENT`: The increment for dynamic re-allocation of arrays.
- `APECSS_STRINGLENGTH`: The standard length of a string.
- `APECSS_STRINGLENGTH_SPRINTF`: The standard length of a string to be written out in the terminal.
- `APECSS_STRINGLENGTH_SPRINTF_LONG`: The standard length of a long string to be written out in the terminal.
- `APECSS_WHERE`: Outputs in the terminal the file name and line number where the macro is called.
- `APECSS_WHERE_INT(a)`: Outputs in the terminal the file name and line number where the macro is called, plus the integer value a .
- `APECSS_WHERE_FLOAT(a)`: Outputs in the terminal the file name and line number where the macro is called, plus the floating point value a .

2.4.2 Structures

Structures (`struct`) are used in APECSS to group variables and functions, and to provide a modular layout of the code that enables reusing different parts of it.

The structure `APECSS_Bubble` is the central structure of APECSS as it contains all the information related to a bubble. There is, of course, no *a priori* limit on how many copies of this structure a simulation can have, for instance, a multi-bubble simulation with 100 bubbles would naturally have 100 objects of type `struct APECSS_Bubble`. Aside from key information about the bubble, such as the bubble radius, the `APECSS_Bubble` structure contains pointers to the properties of the liquid the bubble is immersed in (`struct APECSS_Liquid`), the properties of the gas the bubble contains (`struct APECSS_Gas`) as well as the properties of its interface (`struct APECSS_Interface`). If applicable, the `APECSS_Bubble` structure also points to the structure with the information of the driving acoustic excitation (`struct APECSS_Excitation`), the structure handling the acoustic emissions (`struct APECSS_Emissions`), and the structure containing the desired results (`struct APECSS_Results`).

The (optional) structure `APECSS_Emissions` is, as the name suggests, related to the acoustic emissions of a bubble. If allocated, it contains information about how to handle the acoustic emissions, function pointers referring to the functions used to advance the acoustic emissions using a Lagrangian wave tracking approach and, very importantly, the linked list of emissions nodes (`struct APECSS_EmissionNode`) that carry the actual information of the acoustic emissions. The structure `APECSS_EmissionNode` holds the information (e.g. radial location, velocity, pressure) associated with a specific emission node.

The (optional) structure `APECSS_Results` holds all the results the user may want to have written out. For performance reasons, the results are in general not written to disk on-the-fly, but are stored in arrays and dumped to disk at the end of the simulation. The `APECSS_Results` structure contains optional structures for the results of the Rayleigh-Plesset model (`struct APECSS_ResultsBubble`) and for the acoustic emissions (`APECSS_ResultsEmissions`).

2.4.3 A word on function pointers

APECSS uses function pointers extensively. Function pointers are an elegant means in C to add complexity and functionality yet still retain a slim code, avoid redundant code and, if nothing else, avoid a large number of costly conditional statements. However, function pointers can quickly make a code unreadable and obscure what is actually happening, if they are used without care. In order to

keep the use of function pointers in APECSS transparent, the adopted convention is that all function pointers are set in `apecss*_processoptions()` functions, e.g. `apecss_gas_processoptions()`.

2.4.4 Code formatting

To ensure a consistent formatting, please use a *clang* formatter that formats the file automatically upon saving. The file defining the formatting of the APECSS source code (`.clang-format`) is part of the repository. A *clang* formatter (supported by most IDEs and editors) should be used for contributions to APECSS. The formatter should recognize this `.clang-format` file automatically.

2.5 Important functions

Here we briefly outline how to use some of the key functions of APECSS.

Whenever using APECSS, at least one `APECSS_Bubble` structure has to be available and, if multiple bubbles are part of a simulation, each bubble has to be represented by a separate `APECSS_Bubble` structure. A single `APECSS_Bubble` structure is allocated and initialized as follows:

```
1 struct APECSS_Bubble *Bubble = (struct APECSS_Bubble *) malloc(sizeof(struct
  APECSS_Bubble));
2 apecss_bubble_initializestruct(Bubble);
```

The function `apecss_bubble_initializestruct()` ensures that all pointers (to arrays, other structures and functions) that are part of the `APECSS_Bubble` structure are initialized to `NULL`. This is important because the processing of options and any checks for allocation depend on `NULL` to indicate that a given pointer is not yet allocated or not in use.

Once a `APECSS_Bubble` structure is allocated and initialized, default values ought to be set, the `*.apecss` options file is to be read and the chosen options have to be processed. In the standalone examples found in `$APECSS_DIR/examples` this is done with the following function calls:

```
1 apecss_options_setdefault(Bubble);
2 char OptionsDir[APECSS_STRINGLENGTH];
3 sprintf(OptionsDir, "./run.apecss"); // Relative path to the options file.
4 apecss_options_readfile(Bubble, OptionsDir);
5 apecss_options_process(Bubble);
```

While setting default values is advised, for instance using the function `apecss_options_setdefault()`, it is optional. Processing the given options correctly, however, is critical to the working of APECSS and the using the function `apecss_options_process()` is strongly encouraged.

Now that all options have been read and processed, the bubble has to be initialized based on the given options. This includes, for instance, computing the initial gas density and, if applicable, hardcore radius or co-volume.

```
1 apecss_bubble_initialize(Bubble);
```

The heart of APECSS is, of course, the solver. The solver is split into three separate functions that (i) initialize the solver, (ii) run the solver and (iii) wrap up (i.e. finalize) the solver:

```
1 apecss_bubble_solver_initialize(Bubble);
2 apecss_bubble_solver_run(tend, Bubble);
3 apecss_bubble_solver_finalize(Bubble);
```

The initialization of the solver with `apecss_bubble_solver_initialize()` makes sure all counters, the solution error variable and, if applicable, result variables are initialized correctly. The function `apecss_bubble_solver_run()` contains the time-stepping procedure that executes the solver until a specified end time `tend`, given as the first argument of the function call. In the examples found in `$APECSS_DIR/examples`, the function `apecss_bubble_solver_run()` is only called once with

`tend = Bubble->tEnd`, i.e. the end of the simulation. However, the user is free to call the function `apecss_bubble_solver_run()` an arbitrary number of times, with any meaningful end time. This facilitates coupling APECSS to other numerical software frameworks, where `tend` then could for instance be the end of the next time-step of a fluid dynamics solver. As an example simply chopping the simulation up into five equal-sized parts would look like:

```
1  apecss_bubble_solver_initialize(Bubble);
2  apecss_bubble_solver_run(0.2 * tend, Bubble);
3  apecss_bubble_solver_run(0.4 * tend, Bubble);
4  apecss_bubble_solver_run(0.6 * tend, Bubble);
5  apecss_bubble_solver_run(0.8 * tend, Bubble);
6  apecss_bubble_solver_run(tend, Bubble);
7  apecss_bubble_solver_finalize(Bubble);
```

A solver run is ended with the function `apecss_bubble_solver_finalize()` where, for instance, the arrays and linked list of the acoustic emissions are freed.

```
1  Bubble->Excitation = (struct APECSS_Excitation *) malloc(sizeof(struct
    APECSS_Excitation));
2  Bubble->Excitation->type = APECSS_EXCITATION_SIN;
3  Bubble->Excitation->f = (APECSS_FLOAT) fa;
4  Bubble->Excitation->dp = (APECSS_FLOAT) pa;
```

Chapter 3

Bubble dynamics

The dynamic behaviour of the bubble is modelled with a Rayleigh-Plesset-type (RP) model, assuming spherical symmetry. This requires to choose a suitable RP-type model (Section 3.1) and define appropriate conditions for the gas (Section 3.2), the liquid (Section 3.3), the interface (Section 3.4), as well as at infinity (Section 3.5). The results that APECSS can write out based on the RP model are explained in Section 3.6.

APECSS solves all ordinary differential equations (ODEs) using the embedded RK5(4) scheme of Dormand and Prince [5], whereby a fifth-order Runge-Kutta scheme is used to solve the ODEs and the corresponding fourth-order Runge-Kutta scheme is used to estimate the solution error. Based on this solution error, the time-step Δt used to advance the solution of the ODEs is adapted.

| Section | Command | Description |
|-----------|----------------------------|---|
| BUBBLE | InitialRadius <float> | The initial radius R_0 of the bubble. |
| | PressureAmbient <float> | The ambient pressure p_0 . |
| | InitialGasPressure <float> | The initial gas pressure $p_{G,0}$, if different from p_0 or the corresponding Laplace pressure. |
| ODESOLVER | RK 7M | Minimum truncation (7M) coefficients of the RK5(4) scheme of Dormand and Prince [5]. This is the default. |
| | RK 7S | Stability optimized (7S) coefficients of the RK5(4) scheme of Dormand and Prince [5]. |
| | Tolerance <float> | The desired solution tolerance. |
| | MinTimeStep <float> | Minimum time-step Δt . |
| | MaxTimeStep <float> | Maximum time-step Δt . |
| | MaxSubIterations <float> | Maximum number of sub-iterations in a given time-step. |

3.1 Rayleigh-Plesset models

APECSS offers four RP-type models to simulate pressure-driven bubble dynamics: the standard Rayleigh-Plesset model without and with acoustic radiation damping, the Keller-Miksis model and the Gilmore model.

| Section | Command | Description |
|---------|----------------|---|
| BUBBLE | RPMoel RP | Standard Rayleigh-Plesset model, Eq. (3.1). This is the default. |
| | RPMoel RPAR | Rayleigh-Plesset model including acoustic radiation damping, Eq. (3.2). |
| | RPMoel KM | Keller-Miksis model, Eq. (3.3). |
| | RPMoel Gilmore | Gilmore model, Eq. (3.4). |

The standard Rayleigh-Plesset (RP) model is given as [14]

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 = \frac{p_L - p_\infty}{\rho_{\ell,\text{ref}}}, \quad (3.1)$$

where R is the bubble radius, p_L is the pressure of the liquid at the bubble wall, p_∞ is the pressure of the liquid at infinite distance from the bubble, p_G is the pressure of the gas inside the bubble and $\rho_{\ell,\text{ref}}$ is the *constant* density of the liquid.

To incorporate acoustic radiation in the liquid and the associated damping, the modified Rayleigh-Plesset model is given as [1]

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 = \frac{p_L - p_\infty}{\rho_{\ell,\text{ref}}} + \frac{R\dot{p}_G}{\rho_{\ell,\text{ref}} c_{\ell,\text{ref}}}, \quad (3.2)$$

where $c_{\ell,\text{ref}}$ is the *constant* reference speed of sound of the liquid. The last term on the right-hand side accounts for acoustic radiation in the liquid. This modified RP model is frequently used to simulate medical ultrasound applications [23] as well as sonoluminescence [1]. It follows directly from the Keller-Miksis model, Eq. (3.3), which incorporates the compressibility of the liquid, by assuming the Mach number of the bubble wall is vanishingly small, $M_\ell = \dot{R}/c_{\ell,\text{ref}} \simeq 1$. Eq. (3.2) is, consequently, only valid for small Mach numbers $M_\ell \ll 1$ [17, 19].

The Keller-Miksis model [11, 19], which incorporates the compressibility of the liquid to first order, is given as

$$\left(1 - \frac{\dot{R}}{c_{\ell,\text{ref}}}\right) R\ddot{R} + \frac{3}{2} \left(1 - \frac{\dot{R}}{3c_{\ell,\text{ref}}}\right) \dot{R}^2 = \left(1 + \frac{\dot{R}}{c_{\ell,\text{ref}}}\right) \frac{p_L - p_\infty}{\rho_{\ell,\text{ref}}} + \frac{R\dot{p}_L}{\rho_{\ell,\text{ref}} c_{\ell,\text{ref}}}, \quad (3.3)$$

where $c_{\ell,\text{ref}}$ is the speed of sound of the liquid. Both $\rho_{\ell,\text{ref}}$ and $c_{\ell,\text{ref}}$ are assumed to be constant, limiting the Keller-Miksis model to moderate liquid pressures ($p_L \lesssim 10^8$ Pa).

Based on the Kirkwood-Bethe hypothesis [3, 12], Gilmore [7] derived a second-order ordinary differential equation describing the radial dynamics of a bubble in a compressible liquid,

$$\left(1 - \frac{\dot{R}}{c_L}\right) R\ddot{R} + \frac{3}{2} \left(1 - \frac{\dot{R}}{3c_L}\right) \dot{R}^2 = \left(1 + \frac{\dot{R}}{c_L}\right) H + \left(1 - \frac{\dot{R}}{c_L}\right) \frac{R\dot{H}}{c_L}, \quad (3.4)$$

where c_L is the speed of sound of the liquid at the bubble wall, $H = h_L - h_\infty$ is the enthalpy difference between the bubble wall and infinity, and $\dot{H} = \dot{h}_L - \dot{h}_\infty$ is the derivative of H . The enthalpy h and the speed of sound c are defined by an appropriate equation of state as a function of pressure, with $h_L = h(p_L)$, $h_\infty = h(p_\infty)$ and $c_L = c(p_L)$, as detailed in 3.3.

3.2 The gas

In APECSS, every bubble contains a gas, which requires to select an appropriate equation of state and define meaningful properties.

| Section | Command | Description |
|---------|----------------------------|--|
| GAS | EoS IG | Ideal gas equation of state. This is the default. |
| | EoS HC | Ideal gas equation of state with van-der-Waals hardcore. |
| | EoS NASG | Noble-Abel-stiffened-gas equation of state. |
| | PolytropicExponent <float> | Polytropic exponent Γ_g . |
| | ReferencePressure <float> | Reference pressure $p_{g,\text{ref}}$. |
| | ReferenceDensity <float> | Reference density $\rho_{g,\text{ref}}$. |
| | HardcoreRadius <float> | Hardcore radius r_{hc} . |
| | CoVolume <float> | Co-volume b_g . |
| | TaitPressureConst <float> | Pressure constant B_g . |
| | MolecularWeight <float> | Molecular weight \mathcal{M}_g of the gas. |
| | MolecularDiameter <float> | Molecular kinematic diameter \mathcal{D}_g of the gas. |

Using the ideal gas EoS, the pressure and its derivative are given as

$$p_G = p_{G,\text{ref}} \left(\frac{R_0}{R} \right)^{3\Gamma_g} \quad (3.5)$$

$$\dot{p}_G = -3 \frac{p_G \Gamma_g \dot{R}}{R}, \quad (3.6)$$

$$(3.7)$$

including a van-der-Waals hardcore (HC) in the ideal gas model, the pressure and its derivative follow as

$$p_G = p_{G,\text{ref}} \left(\frac{R_0^3 - r_{\text{hc}}^3}{R^3 - r_{\text{hc}}^3} \right)^{\Gamma_g} \quad (3.8)$$

$$\dot{p}_G = -3 \frac{p_G \Gamma_g R^2 \dot{R}}{R^3 - r_{\text{hc}}^3}, \quad (3.9)$$

and using the Noble-Abel-stiffened-gas (NASG) EoS, the pressure and its derivative are [4]

$$p_G = (p_{G,\text{ref}} + B_g) \left[\frac{\rho_g (1 - b_g \rho_{g,\text{ref}})}{\rho_{g,\text{ref}} (1 - b_g \rho_G)} \right]^{\Gamma_g} - B_g \quad (3.10)$$

$$\dot{p}_G = \frac{\dot{\rho}_G \Gamma_g (p_G + B_g)}{\rho_G (1 - b_g \rho_G)}, \quad (3.11)$$

where Γ_g is the polytropic exponent, r_{hc} is the hardcore radius, b_g is the co-volume and B_g is a pressure constant.

Assuming mass conservation, the gas density and its derivative are given by

$$\rho_G = \rho_{g,\text{ref}} \left(\frac{R_0}{R} \right)^3 \quad (3.12)$$

$$\dot{\rho}_G = -3 \rho_G \frac{\dot{R}}{R}. \quad (3.13)$$

The hardcore radius r_{hc} and the co-volume b_g are set by default to -1 . If the HC or NASG model is chosen, the user has to pass values for the hardcore radius r_{hc} or the co-volume b_g , respectively. Alternatively, the molecular weight \mathcal{M}_g and the molecular kinematic diameter \mathcal{D}_g of the gas may be defined instead of r_{hc} or b_g ; APECSS then computes, based on the bubble size, the correct hardcore radius r_{hc} or co-volume b_g . Based on the molecular weight \mathcal{M}_g , the bubble contains

$$N_G = N_A \frac{\rho_{G,0} V_0}{\mathcal{M}_g} \quad (3.14)$$

molecules, where N_A is the Avogadro constant (see macro `APECSS_AVOGADRO`), $\rho_{G,0}$ is the initial gas density and V_0 is the initial bubble volume. As per the molecular kinetic diameter \mathcal{D}_g of the gas molecules, the volume of each molecule is

$$V_{\text{mol}} = \frac{\pi}{6} \mathcal{D}_g^3. \quad (3.15)$$

The van-der-Waals hardcore radius is then readily defined as

$$r_{\text{hc}} = \sqrt[3]{\frac{3}{4\pi} f_{\text{mol}} V_{\text{mol}} N_G} \quad (3.16)$$

and the co-volume of the gas is given as

$$b_g = f_{\text{mol}} N_A \frac{V_{\text{mol}}}{\mathcal{M}_g}. \quad (3.17)$$

The semi-empirical constant f_{mol} is based on the repulsive forces acting between the molecules [13, 22], and is typically taken to be $f_{\text{mol}} = 4$.

3.3 The liquid

In the same way that every bubble contains a gas, in APECSS every bubble is surrounded by a liquid, which requires to select an appropriate equation of state and fluid type, as well as define meaningful properties.

| Section | Command | Description |
|---------|-------------------------------|---|
| LIQUID | EoS Tait | The Tait EoS is applied to the liquid. Only relevant for the Gilmore model and acoustic emissions based on the Kirkwood-Bethe hypothesis. |
| | EoS NASG | The Noble-Abel-stiffened-gas EoS is applied to the liquid. Only relevant for the Gilmore model and acoustic emissions based on the Kirkwood-Bethe hypothesis. |
| | LiquidType Newtonian | Newtonian fluid. This is the default. |
| | LiquidType KelvinVoigt | Kelvin-Voigt solid. |
| | LiquidType Zener | Zener solid. |
| | LiquidType OldroydB | Oldroyd-B (or upper-convected Maxwell) fluid. |
| | PolytropicExponent <float> | Polytropic exponent Γ_ℓ . |
| | ReferencePressure <float> | Reference pressure $p_{\ell,\text{ref}}$. |
| | ReferenceDensity <float> | Reference density $\rho_{\ell,\text{ref}}$. |
| | ReferenceSpeedofSound <float> | Reference speed of sound $\rho_{\ell,\text{ref}}$. |
| | CoVolume <float> | Co-volume b_ℓ . |
| | TaitPressureConst <float> | Pressure constant B_ℓ . |
| | Viscosity <float> | Newtonian viscosity μ_ℓ . |
| | PolymerViscosity <float> | Polymer viscosity η_ℓ associated with viscoelasticity. |
| | ShearModulus <float> | Shear modulus G_ℓ associated with viscoelasticity. |
| | RelaxationTime <float> | Relaxation time λ_ℓ associated with viscoelasticity. |

The pressure at the bubble wall of a Newtonian liquid is given as

$$p_L = p_G - \frac{2\sigma}{R} - 4\mu_\ell \frac{\dot{R}}{R}, \quad (3.18)$$

where p_G is the gas pressure, see Section 3.2, σ is the surface tension coefficient of the interface, see Section 3.4, and μ_ℓ is the liquid (Newtonian) viscosity. The derivative of Eq. (3.18) follows as

$$\dot{p}_L = \dot{p}_G + \frac{2\sigma\dot{R}}{R^2} + 4\mu_\ell \left(\frac{\dot{R}^2}{R^2} - \frac{\ddot{R}}{R} \right). \quad (3.19)$$

3.3.1 Equation of state

For the Gilmore model (3.4) and the acoustic emissions based on the Kirkwood-Bethe hypothesis (see Section 4.4), an equation of state (EoS) for the liquid has to be defined. Two EoS are currently available in APECSS: the Tait EoS and the NASG EoS.

Since the seminal work of Gilmore [7], the Tait EoS is traditionally used to describe the properties of the liquid in Eq. (3.4). The Tait EoS defines the density ρ , enthalpy h and speed of sound c as

$$\rho = \rho_{\ell,\text{ref}} \left(\frac{p + B_\ell}{p_{\ell,\text{ref}} + B_\ell} \right)^{\frac{1}{\Gamma_\ell}} \quad (3.20)$$

$$h = \frac{\Gamma_\ell}{\Gamma_\ell - 1} \frac{p + B_\ell}{\rho} \quad (3.21)$$

$$c = \sqrt{(\Gamma_\ell - 1)h}, \quad (3.22)$$

respectively, where B_ℓ is a pressure constant, Γ_ℓ is the polytropic exponent, $p_{\ell,\text{ref}}$ is the reference pressure and $\rho_{\ell,\text{ref}}$ is the reference density. For water, typical values are $\Gamma_\ell = 7.15$, $B_\ell = 3.046 \times 10^8$ Pa, $\rho_{\ell,\text{ref}} = 997 \text{ kg/m}^3$ and $p_{\ell,\text{ref}} = 10^5$ Pa. However, the Tait EoS cannot provide physically-meaningful temperature values [20].

Using the Noble-Abel stiffened-gas (NASG) EoS [15] instead of the Tait EoS, the fluid properties are defined as [4]

$$\rho = \frac{K_\ell (p + B_\ell)^{\frac{1}{\Gamma_\ell}}}{1 + b_\ell K_\ell (p + B_\ell)^{\frac{1}{\Gamma_\ell}}} \quad (3.23)$$

$$h = \frac{\Gamma_\ell}{\Gamma_\ell - 1} \frac{p + B_\ell}{\rho} - \frac{\Gamma_\ell b_\ell}{\Gamma_\ell - 1} (p + B_\ell) + b_\ell p \quad (3.24)$$

$$c = \sqrt{\Gamma_\ell \frac{(p + B_\ell)}{\rho - b_\ell \rho^2}}, \quad (3.25)$$

with $K_\ell = \rho_{\ell,\text{ref}} / [(p_{\ell,\text{ref}} + B_\ell)^{1/\Gamma_\ell} (1 - b_\ell \rho_{\ell,\text{ref}})]$ describing a constant reference state, and where b_ℓ is the co-volume of the liquid molecules. The NASG EoS reduces to the Tait EoS for $b_\ell = 0$. Appropriate properties for water have, for instance, been proposed by Chandran and Salih [2] as $\Gamma_\ell = 1.19$, $B_\ell = 6.2178 \times 10^8$ Pa, $b_\ell = 6.7212 \times 10^{-4} \text{ m}^3/\text{kg}$, $\rho_{\ell,\text{ref}} = 997 \text{ kg/m}^3$ and $p_{\ell,\text{ref}} = 10^5$ Pa.

3.3.2 Viscoelasticity

Currently, APECSS supports three widely-used models for viscoelastic media: the Kelvin-Voigt model, the Zener model and the Oldroyd-B model. While the Kelvin-Voigt model merely yields an additional term in the expression for the liquid pressure at the bubble wall, Eq. (3.18), the Zener and Oldroyd-B models each require to solve two additional ODEs.

3.3.2.1 Kelvin-Voigt model

To model a Kelvin-Voigt medium, the elasticity of the medium is modelled by the term

$$\frac{4}{3} G_\ell \frac{R^3 - R_0^3}{R^3}, \quad (3.26)$$

which contributes to Eq. (3.18) to obtain

$$p_L = p_G - \frac{2\sigma}{R} - 4\mu_\ell \frac{\dot{R}}{R} - \frac{4}{3} G_\ell \frac{R^3 - R_0^3}{R^3}, \quad (3.27)$$

where G_ℓ is the elastic shear modulus. The derivative of the liquid pressure at the bubble wall is then given as

$$\dot{p}_L = \dot{p}_G + \frac{2\sigma \dot{R}}{R^2} + 4\mu_\ell \left(\frac{\dot{R}^2}{R^2} - \frac{\ddot{R}}{R} \right) - 4G_\ell \frac{R_0^3 \dot{R}}{R^4}. \quad (3.28)$$

3.3.2.2 Zener model

A more sophisticated viscoelastic model than the Kelvin-Voigt model is the Zener model, also known as standard linear solid model. With the Zener model, the stresses in the medium surrounding the bubble are incorporated in the liquid pressure at the bubble wall as [9]

$$p_L = p_G - \frac{2\sigma}{R} + 3\varsigma \quad (3.29)$$

where

$$\varsigma = \int_R^\infty \frac{\tau_{rr}(r, t)}{r} dr \quad (3.30)$$

is an auxiliary variable associated with the rr -component of the viscous stress tensor $\boldsymbol{\tau}(r, t)$. The auxiliary stress variable is governed by

$$\lambda_\ell \dot{\varsigma} + \varsigma + \lambda_\ell \frac{\dot{R}}{R} \tau_{rr|_R} = -\frac{S}{3}, \quad (3.31)$$

with

$$S = \frac{4}{3} G_\ell \left(1 - \frac{R_0^3}{R^3} \right) + 4\mu_\ell \frac{\dot{R}}{R} \quad (3.32)$$

the combined viscous and elastic contributions, where λ_ℓ is the relaxation time, G_ℓ is the shear modulus and μ_ℓ the viscosity. The stress at the bubble wall, $\tau_{rr|_R}$, evolves as

$$\lambda_\ell \dot{\tau}_{rr|_R} + \tau_{rr|_R} = -S. \quad (3.33)$$

The question is now how to solve the ODEs for ς and τ_{rr} in such a way that we always obtain a meaningful result, even if $\lambda_\ell = 0$. In order for a customary ODE solver to handle this correctly, we rearrange Eqs. (3.31) and (3.33). Under the discrete assumption

$$\dot{\varsigma} = \frac{\varsigma_{n+1} - \varsigma_n}{\Delta t}, \quad (3.34)$$

Eq. (3.31) becomes

$$\lambda_\ell \frac{\varsigma_{n+1} - \varsigma_n}{\Delta t} + \varsigma_{n+1} + \lambda_\ell \frac{\dot{R}}{R} \tau_{rr|_R} = -\frac{S}{3} \quad (3.35)$$

so that, after some further manipulation,

$$\varsigma_{n+1} = \varsigma_n + \Delta t \frac{-\frac{S}{3} - \lambda_\ell \frac{\dot{R}}{R} \tau_{rr|R,n} - \varsigma_n}{\lambda_\ell + \Delta t}. \quad (3.36)$$

Similarly, Eq. (3.33) follows as

$$\tau_{rr|R,n+1} = \tau_{rr|R,n} + \Delta t \frac{-S - \tau_{rr|R,n}}{\lambda_\ell + \Delta t}. \quad (3.37)$$

Even in the limit $\lambda_\ell = 0$, we can now obtain a meaningful answer, that is Eq. (3.36) reduces to

$$\varsigma = -\frac{S}{3}. \quad (3.38)$$

After inserting Eq. (3.38) into Eq. (3.29) we recover the Kelvin-Voigt model. For $\lambda_\ell = 0$, Eq. (3.37) becomes redundant.

3.3.2.3 Oldroyd-B model

The Oldroyd-B model is a widely used constitutive model for viscoelastic fluids. Following the work of Jiménez-Fernández and Crespo [10], the liquid pressure at the bubble wall including the Oldroyd-B model is given as

$$p_L = p_G - \frac{2\sigma}{R} - 4\mu_\ell \frac{\dot{R}}{R} + \mathcal{S}. \quad (3.39)$$

The polymer stress $\mathcal{S} = \mathcal{S}_1 + \mathcal{S}_2$ is split into two constitutive ODEs,

$$\lambda_\ell \dot{\mathcal{S}}_1 + \mathcal{S}_1 + 4\lambda_\ell \frac{\dot{R}}{R} \mathcal{S}_1 = -2\eta_\ell \frac{\dot{R}}{R} \quad (3.40)$$

$$\lambda_\ell \dot{\mathcal{S}}_2 + \mathcal{S}_2 + \lambda_\ell \frac{\dot{R}}{R} \mathcal{S}_2 = -2\eta_\ell \frac{\dot{R}}{R} \quad (3.41)$$

where η_ℓ is the polymer viscosity. These ODEs are reformulated in a similar manner as for the Zener model shown above, to yield

$$\mathcal{S}_{1,n+1} = \mathcal{S}_{1,n} + \Delta t \frac{-\left(4\lambda_\ell \frac{\dot{R}}{R} + 1\right) \mathcal{S}_{1,n} - 2\eta_\ell \frac{\dot{R}}{R}}{\lambda_\ell + \Delta t} \quad (3.42)$$

$$\mathcal{S}_{2,n+1} = \mathcal{S}_{2,n} + \Delta t \frac{-\left(\lambda_\ell \frac{\dot{R}}{R} + 1\right) \mathcal{S}_{2,n} - 2\eta_\ell \frac{\dot{R}}{R}}{\lambda_\ell + \Delta t}. \quad (3.43)$$

For $\lambda_\ell = 0$ Eqs. (3.42) and (3.43) still give a meaningful result and reduce to a Newtonian fluid with $\mathcal{S} = -4\eta_\ell \dot{R}/R$.

3.4 The interface

APECSS readily supports the gas-liquid interface, also often referred to as the *bubble wall*, to be either clean, for which only the surface tension coefficient has to be defined, or coated with a lipid monolayer.

| Section | Command | Description |
|-----------|---------------------------------------|--|
| INTERFACE | SurfaceTensionCoeff <float> | Surface tension coefficient σ_c of the clean interface. |
| | LipidCoatingModel None | No lipid coating model is applied. This is the default. |
| | LipidCoatingModel Marmottant | The lipid coating model of Marmottant <i>et al.</i> [16] is applied. |
| | LipidCoatingModel Gompertz-Marmottant | The continuous variant of the lipid coating model of Marmottant proposed by Gümmer <i>et al.</i> [8] is applied. |
| | SigmaInit <float> | Initial surface tension coefficient σ_0 of the lipid coating model at R_0 . |
| | Elasticity <float> | Elasticity χ of the lipid coating model. |
| | DilatationalViscosity <float> | Dilatational viscosity κ_s of the lipid coating model. |

The influence of surface tension, the rheology of the lipid-monolayer coating and the viscous dissipation in the liquid is accounted for through the definition of the liquid pressure at the bubble wall, given as [16]

$$p_L = p_G - \frac{2\sigma}{R} - 4\mu_\ell \frac{\dot{R}}{R} - 4\kappa_s \frac{\dot{R}}{R^2}, \quad (3.44)$$

where σ is the surface tension coefficient, μ_ℓ is the dynamic viscosity of the liquid and κ_s is the surface dilatational viscosity of the lipid monolayer.

A clean gas-liquid interface has a surface tension coefficient of $\sigma = \sigma_c$ and a surface dilatational viscosity of $\kappa_s = 0$.

Using the model of Marmottant *et al.* [16] to describe a lipid monolayer coating of the interface, the surface tension is defined as

$$\sigma = \begin{cases} 0 & \text{for } R \leq R_{\text{buck}} \\ \chi \left(\frac{R^2}{R_{\text{buck}}^2} - 1 \right) & \text{for } R_{\text{buck}} < R < R_{\text{rupt}} \\ \sigma_c & \text{for } R \geq R_{\text{rupt}} \end{cases} \quad (3.45)$$

where χ is the surface elasticity of the lipid monolayer, the buckling radius is [18]

$$R_{\text{buck}} = \frac{R_0}{\sqrt{1 + \sigma_0/\chi}}, \quad (3.46)$$

where σ_0 is the surface tension coefficient of the lipid-coated bubble at $R = R_0$, and the rupture radius is

$$R_{\text{rupt}} = R_{\text{buck}} \sqrt{1 + \frac{\sigma_c}{\chi}}. \quad (3.47)$$

The radius-dependent surface tension coefficient of the Marmottant model [16], defined in Eq. (3.45), contains two discontinuities at $R = R_{\text{buck}}$ and $R = R_{\text{rupt}}$. These discontinuities render the Marmottant model sensitive to the applied time-step when numerically solving the primary ordinary differential equation [23]. A continuously differentiable form of the Marmottant model a Gompertz function of the form $f(x) = a e^{-b e^{-cx}}$, a special case of the generalized logistics function, was proposed by Gümmer *et al.* [8]. Using this Marmottant-Gompertz model, the surface tension coefficient is defined as

$$\sigma = \sigma_c e^{-b e^{c(1-R/R_{\text{buck}})}}, \quad (3.48)$$

with

$$b = -\frac{\ln(\sigma_0/\sigma_c)}{e^{c(1-R_0/R_{\text{buck}})}} \quad (3.49)$$

and

$$c = \frac{2\chi e}{\sigma_c} \sqrt{1 + \frac{\sigma_c}{2\chi}}. \quad (3.50)$$

The buckling radius R_{buck} is given by Eq. (3.46). The derivative of the surface tension coefficient follows as

$$\dot{\sigma} = \sigma b c e^{c(1-R/R_{\text{buck}})} \frac{\dot{R}}{R}. \quad (3.51)$$

The Marmottant-Gompertz model reproduces the main features of the original Marmottant model [8], but with a smooth transition between the surface tension regimes, using the same set of input parameters (σ_0 , σ_c , χ) as the original Marmottant model.

3.5 Infinity

The pressure at infinity, p_∞ , is used to apply a driving pressure difference for the bubble dynamics. Presently, APECSS readily supports a constant ambient pressure $p_\infty = p_0$, which may also be replaced by a pressure defined on-the-fly, or a sinusoidal excitation.

A sinusoidal excitation is defined as $p_\infty = p_0 - \Delta p_a \sin(2\pi f_a t)$, where f_a and Δp_a are the frequency and pressure amplitude of the excitation. In order to use the sinusoidal excitation, the user has to allocate the pointer `*Excitation`, in the structure `APECSS_Bubble` structure, with `struct APECSS_Excitation` and define the desired values for f_a and Δp_a . The example found in the folder `example/ultrasound/` provides a template of how to do this.

3.6 Results

The results of the bubble dynamics can be written to disk, if the user wants that. Note that APECSS does not write any results to disk unless it is specifically ask to do so.

| Section | Command | Description |
|---------|--|---|
| RESULTS | <code>Bubble</code> | Results of the bubble dynamics are written to file. |
| | <code>OutputFreqRP <int></code> | Results of the bubble dynamics are stored every so many time steps (default: 1). |
| | <code>OutputPath <string></code> | Path to the folder where all the results should be written in to (default: <code>./</code>). |
| | <code>OutputDigits <int></code> | Results are written out with as many digits (default: 6). |

For the bubble dynamics, the following quantities as a function of time are written into a text file, named by the employed RP model and (if applicable) the excitation parameters used:

- Time-step number.
- Time, t .
- Time-step, Δt .
- Bubble radius, R .
- Velocity of the bubble wall, \dot{R} .

- Pressure of the gas, p_G .
- Pressure of the liquid at the bubble wall, p_L .
- Speed of sound of the liquid at the bubble wall, c_L , if the Gilmore model is applied.
- The result of any additional user-defined ODE solved, if applicable.

The first line of the results file(s) lists the variables that were written out and their order.

Chapter 4

Acoustic emissions

Modeling the acoustic emissions is a core feature of APECSS. To this end, APECSS offers different models for the acoustic emissions, assuming an incompressible liquid, a weakly-compressible liquid or a fully-compressible liquid. To account for a finite propagation speed, the information associated with an emitted acoustic wave is propagated along the radial coordinate axis using a Lagrangian wave tracking approach. Unless specifically told to do so, APECSS does not compute any acoustic emissions.

| Section | Command | Description |
|---------|--------------------------|--|
| BUBBLE | Emissions Incompressible | Computes the acoustic emissions under the common incompressible assumption. |
| | Emissions FTI | Computes the acoustic emissions under the assumption of an incompressible fluid but propagating the emissions with the speed of sound. |
| | Emissions QA | Computes the acoustic emissions using the quasi-acoustic model of Gilmore [7]. |
| | Emissions KB | Computes the acoustic emissions based on the Kirkwood-Bethe hypothesis. |

4.1 Lagrangian wave tracking

APECSS tracks acoustic emissions using a Lagrangian wave tracking approach, illustrated in Figure 4.1, in which so-called *emission nodes* are propagated in the radial direction with propagation speed \mathcal{C} . Each emission node, represented in APECSS as a structure `struct APECSS_EmissionNode` and part of a linked list of these structures, holds the current radial coordinate $r(t)$, the flow velocity $u(r, t)$, the pressure $p(r, t)$, the enthalpy $h(r, t)$ if applicable, as well as the invariants $f(\tau)$ and $g(\tau)$ computed based on the solution of the RP model. The definition of the propagation speed \mathcal{C} depends on the chosen model.

The radial position of an emission node at time t is given as

$$r(t) = R(\tau) + \int_{\tau}^t \mathcal{C} \, dt \approx R(\tau) + \sum_{i=1}^N \mathcal{C}(r(t_i), t_i) \Delta t_i, \quad (4.1)$$

where Δt is the numerical time-step and N is the number of time-steps making up the time interval from τ to t .

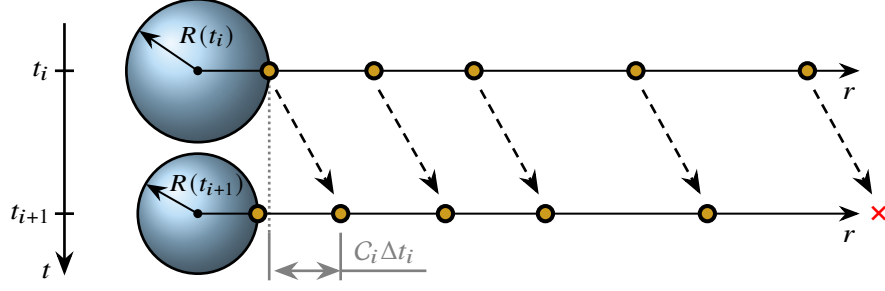


Figure 4.1: Illustration of the Lagrangian transport of the emission nodes, updated at each discrete time instance t_i . Nodes that pass a predefined maximum radial coordinate are discarded.

4.2 Incompressible assumption

Assuming an incompressible liquid ($c_{\ell,\text{ref}} \rightarrow \infty$) with density $\rho_{\ell,\text{ref}}$, the velocity $u(r, t)$ and pressure $p(r, t)$ at a given radial location $r(t)$ are defined as [17]

$$u(r, t) = \frac{R(t)^2 \dot{R}(t)}{r^2} \quad (4.2)$$

and

$$p(r, t) = p_\infty(t) + \rho_{\ell,\text{ref}} \left[\frac{R(t)^2 \ddot{R}(t) + 2 R(t) \dot{R}(t)^2}{r} - \frac{R(t)^4 \dot{R}(t)^2}{2 r^4} \right], \quad (4.3)$$

respectively. The assumption of an incompressible fluid is consistent with the Rayleigh-Plesset models in Eqs. (3.1) and (3.2). Note that, because $\mathcal{C} \rightarrow \infty$, these simple incompressible acoustic emissions do not use the Lagrangian wave tracking and no emission nodes are defined and processed, since pressure and velocity are defined instantaneously for all r .

Alternatively, APECSS also supports the assumption that the liquid is incompressible but the information associated with the acoustic emissions still propagates with finite speed $\mathcal{C} = c_{\ell,\text{ref}}$ using the Lagrangian wave tracking approach. The radial location is then given as

$$r(t) \approx R(\tau) + c_{\ell,\text{ref}} \sum_{i=1}^N \Delta t_{i-1}. \quad (4.4)$$

This approach, referred to in APECSS as FTI or finite-time incompressible, accurately recovers the time delay between emitting information at the bubble wall and this information arriving in a certain location.

4.3 Quasi-acoustic model

Assuming the liquid is compressible but accurately described by a constant density $\rho_{\ell,\text{ref}}$ and constant speed of sound $c_{\ell,\text{ref}}$, Gilmore [7] derived the *quasi-acoustic model* for the acoustic emissions. With the quasi-acoustic model, the velocity, pressure and radial location follows as

$$u(r, t) = \frac{f(\tau)}{r(t)^2} + \frac{g(\tau)}{r(t) c_{\ell,\text{ref}}} \quad (4.5)$$

$$p(r, t) = p_\infty(t) + \rho_{\ell,\text{ref}} \left[\frac{g(\tau)}{r(t)} - \frac{u(r, t)^2}{2} \right] \quad (4.6)$$

$$r(t) \approx R(\tau) + c_{\ell,\text{ref}} \sum_{i=1}^N \Delta t_{i-1}, \quad (4.7)$$

where $f(\tau)$ and $g(\tau)$ are invariants defined based on the result of the employed RP model as

$$f(\tau) = R(\tau)^2 \dot{R}(\tau) - \frac{R(\tau)g(\tau)}{c_{\ell,\text{ref}}} \quad (4.8)$$

$$g(\tau) = R(\tau) \left[\frac{p_L(\tau) - p_\infty}{\rho_{\ell,\text{ref}}} + \frac{\dot{R}(\tau)^2}{2} \right], \quad (4.9)$$

and τ is the time at which the acoustic wave is emitted at the bubble wall. For $t = \tau$ with $r = R(\tau)$, Eq. (4.5) reduces to $u(R, \tau) = \dot{R}(\tau)$ and Eq. (4.6) reduces to $p(R, \tau) = p_L(\tau)$, thus satisfying the boundary conditions at the bubble wall.

The quasi-acoustic model is consistent in its modelling assumptions with the Keller-Miksis model, Eq. (3.3). The applicability of the quasi-acoustic model is limited to small Mach numbers, $(\dot{R}/c_0)^2 \ll 1$, as it incorporates a finite propagation speed of the acoustic emissions and the nonlinear pressure contributions resulting from the flow, but since all parts of the wave propagate with speed c_0 , the quasi-acoustic model can neither describe the nonlinear distortion of acoustic waves nor the formation of shock fronts.

4.4 Emissions based on the Kirkwood-Bethe hypothesis

Following a similar derivation as for the quasi-acoustic model discussed in Section 4.3, but assuming a fully-compressible liquid described by a suitable equation of state, a model for the acoustic emissions based on the Kirkwood-Bethe hypothesis [3, 12] can be derived. With $\mathcal{C}(r, t) = c(r, t) + u(r, t)$, the velocity, enthalpy and radial location of an emission node are then given as

$$u(r, t) = \frac{f(\tau)}{r(t)^2} + \frac{g(\tau)}{r(t) [c(r, t) + u(r, t)]} \quad (4.10)$$

$$h(r, t) = h_\infty(t) + \frac{g(\tau)}{r(t)} - \frac{u(r, t)^2}{2}. \quad (4.11)$$

$$r(t) \approx R(\tau) + \sum_{i=1}^N [c(r(t_i), t_i) + u(r(t_i), t_i)] \Delta t_i, \quad (4.12)$$

where τ is the time at which the acoustic wave is emitted at the bubble wall. The invariants $f(\tau)$ and $g(\tau)$ are defined as

$$f(\tau) = R(\tau)^2 \dot{R}(\tau) - \frac{R(\tau)g(\tau)}{c_L(\tau) + \dot{R}(\tau)} \quad (4.13)$$

$$g(\tau) = R(\tau) \left[h_L(\tau) - h_\infty(\tau) + \frac{\dot{R}(\tau)^2}{2} \right], \quad (4.14)$$

For $t = \tau$ with $r = R(\tau)$, Eq. (4.10) reduces to $u(R, \tau) = \dot{R}(\tau)$ and Eq. (4.11) reduces to $h(R, \tau) = h_L(\tau)$, thus satisfying the boundary conditions at the bubble wall. The pressure $p(r, t)$ can then be readily computed based on the employed equation of state from the enthalpy $h(r, t)$. The assumptions used to derive this model for the acoustic emissions are consistent with the Gilmore model, Eq. (3.4).

Emission nodes with a higher pressure propagate faster than nodes with a lower pressure, which in turn leads to progressive steepening of the acoustic wave. As a result, an emission node may overtake the forerunning emission node, yielding an unphysical multivalued solution. In reality, such a multivalued solution is avoided by the formation of a shock front [6]. Rudnick [21] postulated that the rate of attenuation of a stable shock front is independent of the dissipation process leading to the stable shock front. Exploiting Rudnick's argument, an emission node that overtakes its forerunning neighbor is simply discarded, see Fig. 4.2, thus maintaining a physically plausible solution.

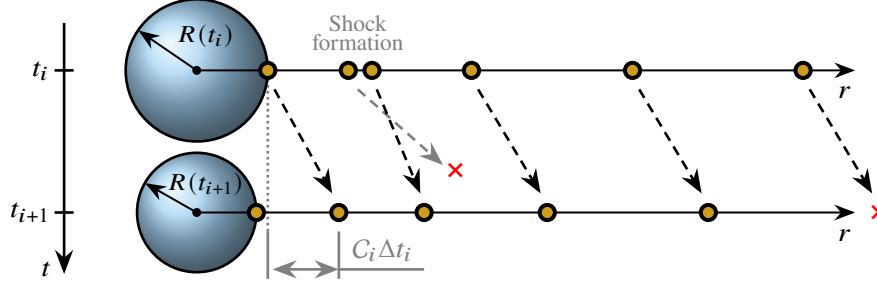


Figure 4.2: Illustration of the Lagrangian transport of the emission nodes, updated at each discrete time instance t_i . Nodes that either overtake the forerunning node, which represents the formation of a shock front, or that pass a predefined maximum radial coordinate are discarded.

4.5 Results

APECSS can write out different results based on the acoustic emissions. Note that APECSS does not write any results to disk unless it is specifically ask to do so.

The acoustic emissions can be recorded as a function of time at one or multiple radial locations (cf. `EmissionsSpace`), or the emissions are written out with respect to their radial location at one or multiple time instances (cf. `EmissionsTime`) or emission nodes (cf. `EmissionsNode`), or for selected extrema in a specified period (cf. `EmissionsMinMax`). This calls can be used multiple times to defined, for instance, multiple radial locations or time instances.

| Section | Command | Description |
|---------|---|--|
| RESULTS | <code>OutputPath <string></code> | Path to the folder where all the results should be written in to (default: <code>./</code>). |
| | <code>OutputDigits <int></code> | Results are written out with as many digits (default: 6). |
| | <code>EmissionsSpace <float></code> | Defines a radial location at which the emissions in the liquid are written out as a function of time. If/while the location is in the gas phase, 0 is recorded. |
| | <code>OutputFreqEmissionsSpace <int></code> | Results of the emissions at a specific radial location are stored every so many time steps (default: 1). |
| | <code>EmissionsTime <float></code> | Defines a time instance at which the emission in the liquid are written out as a function of the radial coordinate. |
| | <code>EmissionsNode <int></code> | Defines a node ID of which the emission in the liquid are written out as a function of the radial coordinate. |
| | <code>EmissionsMinMax <int></code> | Defines the period in which the emission in the liquid are written out as a function of the radial coordinate for the node representing R_{\min} , \dot{R}_{\min} and $p_{L,\max}$. |

The first line of the results file(s) lists the variables that were written out and their order.

Bibliography

- [1] Brenner, M. P., Hilgenfeldt, S., and Lohse, D. (2002). Single-bubble sonoluminescence. *Reviews of Modern Physics*, **74**(2), 425–484.
- [2] Chandran, J. and Salih, A. (2019). A modified equation of state for water for a wide range of pressure and the concept of water shock tube. *Fluid Phase Equilibria*, **483**, 182–188.
- [3] Cole, R. H. (1948). *Underwater Explosions*. Princeton University Press, Princeton, New Jersey.
- [4] Denner, F. (2021). The Gilmore-NASG model to predict single-bubble cavitation in compressible liquids. *Ultrasonics Sonochemistry*, **70**, 105307.
- [5] Dormand, J. and Prince, P. (1980). A family of embedded Runge-Kutta formulae. *Journal of Computational and Applied Mathematics*, **6**(1), 19–26.
- [6] Fay, R. D. (1931). Plane sound waves of finite amplitude. *The Journal of the Acoustical Society of America*, **3**(2A), 222–241.
- [7] Gilmore, F. R. (1952). The growth or collapse of a spherical bubble in a viscous compressible liquid. Technical Report 26-4, California Institute of Technology, Pasadena, California, USA.
- [8] Gümmer, J., Schenke, S., and Denner, F. (2021). Modelling Lipid-Coated Microbubbles in Focused Ultrasound Applications at Subresonance Frequencies. *Ultrasound in Medicine & Biology*, **47**(10), 2958–2979.
- [9] Hua, C. and Johnsen, E. (2013). Nonlinear oscillations following the Rayleigh collapse of a gas bubble in a linear viscoelastic (tissue-like) medium. *Physics of Fluids*, **25**(8), 083101.
- [10] Jiménez-Fernández, J. and Crespo, A. (2005). Bubble oscillation and inertial cavitation in viscoelastic fluids. *Ultrasonics*, **43**(8), 643–651.
- [11] Keller, J. B. and Miksis, M. (1980). Bubble oscillations of large amplitude. *The Journal of the Acoustical Society of America*, **68**(2), 628–633.
- [12] Kirkwood, J. G. and Bethe, H. A. (1942). The pressure wave produced by an underwater explosion. Technical Report 588, Office of Scientific Research and Development.
- [13] Kontogeorgis, G. M., Privat, R., and Jaubert, J.-N. (2019). Taking Another Look at the van der Waals Equation of State—Almost 150 Years Later. *Journal of Chemical & Engineering Data*, **64**(11), 4619–4637.
- [14] Lauterborn, W. and Kurz, T. (2010). Physics of bubble oscillations. *Reports on Progress in Physics*, **73**(10), 106501.
- [15] Le Métayer, O. and Saurel, R. (2016). The Noble-Abel Stiffened-Gas equation of state. *Physics of Fluids*, **28**(4), 046102.
- [16] Marmottant, P., van der Meer, S., Emmer, M., Versluis, M., de Jong, N., Hilgenfeldt, S., and Lohse, D. (2005). A model for large amplitude oscillations of coated bubbles accounting for buckling and rupture. *The Journal of the Acoustical Society of America*, **118**(6), 3499–3505.

- [17] Neppiras, E. A. (1980). Acoustic cavitation. *Physics Reports*, **61**(3), 159–251.
- [18] Overvelde, M., Garbin, V., Sijl, J., Dollet, B., de Jong, N., Lohse, D., and Versluis, M. (2010). Nonlinear Shell Behavior of Phospholipid-Coated Microbubbles. *Ultrasound in Medicine & Biology*, **36**(12), 2080–2092.
- [19] Prosperetti, A. and Lezzi, A. (1986). Bubble dynamics in a compressible liquid. Part 1. First-order theory. *Journal of Fluid Mechanics*, **168**, 457–478.
- [20] Radulescu, M. I. (2020). Compressible flow in a Noble–Abel stiffened gas fluid. *Physics of Fluids*, **32**(5), 056101.
- [21] Rudnick, I. (1952). Theory of the Attenuation of Very High Amplitude Sound Waves. Technical report, Soundrive Engine Company, Los Angeles, California, USA.
- [22] van der Waals, J. (1998). The equation of state for gases and liquids. In S. Lundqvist, editor, *Nobel Lectures in Physics (1901-1921)*, pages 254–265. World Scientific, Singapore.
- [23] Versluis, M., Stride, E., Lajoinie, G., Dollet, B., and Segers, T. (2020). Ultrasound Contrast Agent Modeling: A Review. *Ultrasound in Medicine & Biology*, **46**(9), 2117–2144.