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GENERIC-MOTIVATED EXTENDED SYMPLECTIC NUMERICAL METHODS FOR DISSIPATIVE MECHANICAL SYSTEMS: A CONCRETE EXAMPLE AND GENERAL MESSAGES

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Abstract. The GENERIC (General Equation for the Non-Equilibrium Reversible–Irreversible Coupling) framework is used, first, to present the irreversible thermodynamical formulation of the Rayleigh potential, and, subsequently, to realize the dynamical equations of motion of a supercritical van der Waals fluid separated from the environment by a movable rigid piston. Motivated by the latter, a quasi-symplectic generalization of the symplectic Euler finite-difference numerical scheme is introduced for this setup. A remarkable advantage over the explicit Euler scheme regarding artificial numerical antidissipation is illustrated. The possibility of controlled artificial numerical damping is addressed. The quasi-symplectic scheme is proven to enable efficient simulation of the considerably nonlinear and sensitive processes near the liquid–vapour critical point. A numerically feasible quantitative measure of nonlinearity of time-dependent processes is introduced and applied.

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1. Introduction

For most dynamical systems, in particular nonlinear ones and dissipative ones, solutions are achievable only numerically. Numerical approximations result in a kind of distortion of the original system and introduce the possibility of

- artificial instability (when the solution diverges with exponentially increasing oscillation),
- dissipation or antidissipation error (energies and amplitudes artificially decreasing or increasing), and

- dispersion error (artificial oscillations emerging at sudden spatial or temporal changes).

Instability ruins the solution completely, artificial (anti)dissipation falsifies the true irreversible dissipation of the system, and true oscillations are difficult to distinguish from artificially emerging oscillations.

Choosing a higher-order numerical scheme may not help in these aspects – for instance, with the 4th-order Runge–Kutta method, energy gradually drifts away from the correct value (see,*e.g.,* [1, 2]) and so does the solution as well.

For reversible Hamiltonian systems, a well-established family of trustworthy numerical schemes is the so-called symplectic schemes (see, *e.g.,* [3]). These methods provide outstanding solutions for large simulated times, since a symplectic scheme actually provides the *exact* solution of a nearby Hamiltonian system. Seminal examples are the symplectic Euler method (the symplectic variant of the explicit Euler one), the Störmer–Verlet method, and the symplectic Runge–Kutta methods. The explicit leapfrog method, popular in molecular dynamics for example, is in fact the Störmer–Verlet method for a Hamiltonian in which kinetic energy depends on only some of the phase-space variables while the potential energy depends only on the rest of the variables.

For dissipative, irreversible, systems, the situation is much less developed (see, *e.g.,* [4]). Also, even for reversible cases it is frequently found advantageous to introduce some irreversibility to damp some of the degrees of freedom – those which only play a minor role in the solution but following which requires very fine discretization and, correspondingly, considerable computational resources. Accordingly, there is a multisided need for efficient numerical treatment of – artificially or inherently – irreversible situations.

Now, the native framework for treating irreversible systems is thermodynamics – where thermodynamics is understood in the modern dynamical sense. If a dissipative system is conceived in the whole thermodynamical picture, then one can avoid adhoc or partial solutions to the challenges and can have a globally consistent approach. Following the thermodynamics-related additional quantities extends the treatment to a consistent whole and, by monitoring what happens in regard of the Second Law of Thermodynamics, one can see the contribution of each degree of freedom to irreversibility.

Giving account of irreversibility, as well as its coupling to reversible, *e.g.,* mechanical, properties, has serious technological importance. Just one example is supercritical processes, where one can avoid the disadvantages of phase transition but must be careful when being above the critical point where the material possesses strong nonlinearities and sensitivities (see, *e.g.,* [5]).

The symplectic structure of Hamiltonian reversible systems, and thus the possibility to apply symplectic numerical methods, is lost for irreversible cases, but fortunately only partially. The framework running under the acronym GENERIC (which stands for General Equation for the Non-Equilibrium Reversible–Irreversible Coupling) [6–10] restores as much as possible.

Regarding numerical solutions, following a few pioneering works (see, *e.g.,* [11–13]), a program-announcing article is by Shang and Öttinger [14], where a strategy is introduced to preserve qualities from symplectic methods as much as possible, respecting the structure of GENERIC.

After our earlier works where thermodynamical consistency (for balances, state quantities, and the Second Law of Thermodynamics) and resulting benefits have been utilized for irreversible processes [15–18], here we take a further step by presenting a GENERIC-motivated quasi-symplectic numerical scheme.

We start with a presentation of GENERIC along the example of the Rayleigh potential. Next, we summarize the process-oriented dynamical viewpoint of thermodynamics. Then we present a dynamical setup involving a supercritical fluid and construct the GENERIC formulation of the problem. This is followed by more detailed information about symplectic numerical methods for reversible Hamiltonian systems. Then we introduce our quasi-symplectic scheme on our example setup. Four applications follow:

- comparison between the explicit Euler scheme and ours for the reversible but non-Hamiltonian case,
- a test of how the explicit Euler result can be improved via artificial damping,
- comparison of the quasi-symplectic numerical solutions without damping vs. with damping, and
- analysis of the nonlinearity of the process and the influence of the critical point.

Finally, various lessons are drawn in the Conclusion.

2. Introducing GENERIC along the case of the Rayleigh potential

We start with a simple illustration of how, from mechanics, one can arrive at GENERIC.

2.1. The motion of a point particle with mass m is described (with respect to an inertial reference frame) by its position vector $\mathbf{r}$ as the function of time t, its velocity $\mathbf{v}$ is related to the motion as $\mathbf{v}(t) = \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}$, the momentum of the particle is defined as

$$\mathbf{p} = m\mathbf{v}, \tag{2.1}$$

and its kinetic energy is

$$K = \frac{m}{2}\mathbf{v}^2 = \frac{1}{2m}\mathbf{p}^2. \tag{2.2}$$

Under the influence of a force field $\mathbf{F}(\mathbf{r})$, the motion of the particle satisfies, according to Newton's law:

$$m\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = \mathbf{F}(\mathbf{r}), \qquad m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathbf{F}(\mathbf{r}), \qquad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \mathbf{F}(\mathbf{r}). \tag{2.3}$$

Consequently, along a motion, kinetic energy turns out to fulfil

$$\frac{\mathrm{d}K}{\mathrm{d}t} = \mathbf{F}(\mathbf{r})\mathbf{v} = \mathbf{F}(\mathbf{r})\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}; \tag{2.4}$$

i.e., the rate of change of the kinetic energy equals the power exerted by the force.

In case of a conservative force field, *i.e.,* when $\mathbf{F}$ can be connected to the gradient of a potential as $\mathbf{F}(\mathbf{r}) = -\frac{\mathrm{d}U}{\mathrm{d}\mathbf{r}}$, we have, along a motion,

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\mathrm{d}U}{\mathrm{d}\mathbf{r}}, \tag{2.5}$$

where $\frac{\mathrm{d}\dots}{\mathrm{d}\mathbf{r}}$ denotes the gradient with respect to the vector variable $\mathbf{r}$, together with

$$\frac{\mathrm{d}K}{\mathrm{d}t} = -\frac{\mathrm{d}U}{\mathrm{d}\mathbf{r}}\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\frac{\mathrm{d}U\big(\mathbf{r}(t)\big)}{\mathrm{d}t} \qquad \Longrightarrow \qquad \frac{\mathrm{d}(K+U)}{\mathrm{d}t} = 0. \tag{2.6}$$

In other words, mechanical energy, $E_{\mathrm{mech}} = K + U$, is conserved along a motion.

2.2. Since this is a conservative system, its Newtonian description admits an equivalent formulation based on the Lagrangian

$$L(\mathbf{r}, \mathbf{v}) = K(\mathbf{v}) - U(\mathbf{r}) : \tag{2.7}$$

the Newtonian equation of motion (2.3) is equivalent to that, along a motion,

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \mathbf{v}} = \frac{\partial L}{\partial \mathbf{r}} \tag{2.8}$$

(partial derivatives with respect to vectorial variables still denoting the appropriate gradients), understood together with $\mathbf{v}(t) = \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}$.

Yet another equivalent formulation is based on the Hamiltonian (the Legendre transform of L in its second variable)

$$H(\mathbf{r}, \mathbf{p}) = \frac{\partial L}{\partial \mathbf{v}}\mathbf{v} - L = \mathbf{p}\mathbf{v} - L = K + U, \tag{2.9}$$

which actually embodies mechanical energy in the variables $\mathbf{r}, \mathbf{p}$. In this version, the motion satisfies the set of first-order differential equations

$$\left.\begin{aligned} \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} &= \frac{\partial H}{\partial \mathbf{p}}, \\ \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} &= -\frac{\partial H}{\partial \mathbf{r}}, \end{aligned}\right\} \qquad \text{which can also be written as} \quad \frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\mathbf{r}\\ \mathbf{p}\end{pmatrix} = \begin{pmatrix}\mathbf{0} & \mathbf{1}\\ -\mathbf{1} & \mathbf{0}\end{pmatrix}\begin{pmatrix}\frac{\partial H}{\partial \mathbf{r}}\\ \frac{\partial H}{\partial \mathbf{p}}\end{pmatrix}, \tag{2.10}$$

where $\mathbf{0}$ and $\mathbf{1}$ are the zero and unit tensor, respectively. For the collection of variables $\boldsymbol{x}$, and with $\boldsymbol{\Omega}$, introduced respectively as

$$\boldsymbol{x} = \begin{pmatrix}\mathbf{r}\\ \mathbf{p}\end{pmatrix}, \quad \boldsymbol{\Omega} = \begin{pmatrix}\mathbf{0} & \mathbf{1}\\ -\mathbf{1} & \mathbf{0}\end{pmatrix}, \qquad \text{and with the consequence} \quad \frac{\mathrm{d}H}{\mathrm{d}\boldsymbol{x}} = \begin{pmatrix}\frac{\partial H}{\partial \mathbf{r}}\\ \frac{\partial H}{\partial \mathbf{p}}\end{pmatrix}, \tag{2.11}$$

(2.10) gains the compact form[1]

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{\Omega}\frac{\mathrm{d}H}{\mathrm{d}\boldsymbol{x}}, \qquad \text{rewritten for further purposes as} \qquad \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{\Omega}\frac{\mathrm{d}E_{\mathrm{mech}}}{\mathrm{d}\boldsymbol{x}}. \tag{2.12}$$

2.3. Now let us have an additional, damping-type, force, which is proportional to velocity: then the total force is

$$\mathbf{F}_{\mathrm{tot}} = -\frac{\mathrm{d}U}{\mathrm{d}\mathbf{r}} - \xi\mathbf{v} = -\frac{\mathrm{d}U}{\mathrm{d}\mathbf{r}} - \frac{\xi}{m}\mathbf{p} \tag{2.13}$$

with positive constant coefficient ξ. In this case, mechanical energy is not conserved but is dissipated (decreases) along processes:

$$\frac{\mathrm{d}E_{\mathrm{mech}}}{\mathrm{d}t} = \frac{\mathrm{d}(K+U)}{\mathrm{d}t} = \mathbf{F}_{\mathrm{tot}}\mathbf{v} + \frac{\mathrm{d}U}{\mathrm{d}\mathbf{r}}\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\frac{\mathrm{d}U}{\mathrm{d}\mathbf{r}}\mathbf{v} - \xi\mathbf{v}^2 + \frac{\mathrm{d}U}{\mathrm{d}\mathbf{r}}\mathbf{v} = -\xi\mathbf{v}^2 = -\frac{\xi}{m^2}\mathbf{p}^2. \tag{2.14}$$

2.4. Motivated by the benefits of writing a conservative force as a gradient, following Rayleigh, let us write the damping force $-\xi\mathbf{v}$, with the aid of the dissipation potential

$$D = \frac{\xi}{2}\mathbf{v}^2 = \frac{\xi}{2m^2}\mathbf{p}^2, \tag{2.15}$$

also as a gradient – now a gradient with respect to velocity; hence, Newton's equation reads

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathbf{F}(\mathbf{r},\mathbf{v}) = -\frac{\mathrm{d}U}{\mathrm{d}\mathbf{r}} - \frac{\mathrm{d}D}{\mathrm{d}\mathbf{v}}. \tag{2.16}$$

The two other equivalent formulations now read

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \mathbf{v}} = \frac{\partial L}{\partial \mathbf{r}} - \frac{\mathrm{d}D}{\mathrm{d}\mathbf{v}}; \tag{2.17}$$

$$\begin{aligned} \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} &= \frac{\partial E_{\mathrm{mech}}}{\partial \mathbf{p}}, \\ \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} &= -\frac{\partial E_{\mathrm{mech}}}{\partial \mathbf{r}} - \frac{\mathrm{d}D}{\mathrm{d}\mathbf{v}} = -\frac{\partial E_{\mathrm{mech}}}{\partial \mathbf{r}} - m\frac{\mathrm{d}D}{\mathrm{d}\mathbf{p}}. \end{aligned} \tag{2.18}$$

[1] As a comment, $\boldsymbol{\Omega}$ is a so-called symplectic (*i.e.,* antisymmetric and nondegenerate) cotensor on the phase space – the set of possible values of the collection of variables $\boldsymbol{x} = \begin{pmatrix}\mathbf{r}\\ \mathbf{p}\end{pmatrix}$ (which set is a six-dimensional vector space) – and induces a corresponding symplectic structure, a conserved (time-independent) antisymmetric nondegenerate two-cotensor field on the set of the solutions of (2.12) (which set is a six-dimensional smooth manifold).

The latter can be brought into a compact form analogous to (2.12):

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\mathbf{r}\\ \mathbf{p}\end{pmatrix} = \begin{pmatrix}\mathbf{0} & \mathbf{1}\\ -\mathbf{1} & \mathbf{0}\end{pmatrix}\begin{pmatrix}\frac{\partial E_{\mathrm{mech}}}{\partial \mathbf{r}}\\ \frac{\partial E_{\mathrm{mech}}}{\partial \mathbf{p}}\end{pmatrix} - \begin{pmatrix}\mathbf{0}\\ \frac{\partial D}{\partial \mathbf{v}}\end{pmatrix} = \boldsymbol{\Omega}\frac{\mathrm{d}E_{\mathrm{mech}}}{\mathrm{d}\boldsymbol{x}} - \begin{pmatrix}\mathbf{0}\\ m\frac{\partial D}{\partial \mathbf{p}}\end{pmatrix} = \boldsymbol{\Omega}\frac{\mathrm{d}E_{\mathrm{mech}}}{\mathrm{d}\boldsymbol{x}} - \frac{\mathrm{d}(mD)}{\mathrm{d}\boldsymbol{x}}, \tag{2.19}$$

which, for future purposes, is worth writing also as

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{\Omega}\frac{\mathrm{d}E_{\mathrm{mech}}}{\mathrm{d}\boldsymbol{x}} - \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{x}}\underbrace{\left[\frac{1}{2}\begin{pmatrix}\mathbf{r} & \mathbf{p}\end{pmatrix}\begin{pmatrix}\mathbf{0} & \mathbf{0}\\ \mathbf{0} & \frac{\xi}{m}\mathbf{1}\end{pmatrix}\begin{pmatrix}\mathbf{r}\\ \mathbf{p}\end{pmatrix}\right]}_{mD} = \boldsymbol{\Omega}\frac{\mathrm{d}E_{\mathrm{mech}}}{\mathrm{d}\boldsymbol{x}} - \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{x}}\left[\frac{1}{2}\boldsymbol{x}^{\mathrm{transp}}\begin{pmatrix}\mathbf{0} & \mathbf{0}\\ \mathbf{0} & \frac{\xi}{m}\mathbf{1}\end{pmatrix}\boldsymbol{x}\right]. \tag{2.20}$$

The only aspect missing is a description of the conservation of energy. Namely, we can anticipate – and thermodynamical experience encourages us in this – that a certain total energy is still conserved and the lost mechanical energy is just converted into some other type of energy.

2.5. A minimal modification for this is that we assume a single further type of energy E_{int} (referring to "internal energy") with which $E_{\mathrm{mech}} + E_{\mathrm{int}}$ is conserved, and that the corresponding additional degree of freedom of the system is E_{int} directly. Namely, our collection of variables is increased to

$$\boldsymbol{x} = \begin{pmatrix}\mathbf{r}\\ \mathbf{p}\\ E_{\mathrm{int}}\end{pmatrix}, \tag{2.21}$$

with which total energy is

$$E_{\mathrm{tot}}(\boldsymbol{x}) = K(\mathbf{p}) + U(\mathbf{r}) + E_{\mathrm{int}}, \tag{2.22}$$

also implying

$$\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}} = \begin{pmatrix}\frac{\partial E_{\mathrm{tot}}}{\partial \mathbf{r}}\\ \frac{\partial E_{\mathrm{tot}}}{\partial \mathbf{p}}\\ \frac{\partial E_{\mathrm{tot}}}{\partial E_{\mathrm{int}}}\end{pmatrix} = \begin{pmatrix}\frac{\partial U}{\partial \mathbf{r}}\\ \frac{\partial K}{\partial \mathbf{p}}\\ 1\end{pmatrix} = \begin{pmatrix}\frac{\partial U}{\partial \mathbf{r}}\\ \frac{1}{m}\mathbf{p}\\ 1\end{pmatrix}. \tag{2.23}$$

Along a motion, E_{int} is supposed to increase with the same rate E_{mech} decreases with: in virtue of (2.14),

$$\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}t} = \frac{\xi}{m^2}\mathbf{p}^2. \tag{2.24}$$

The question is whether we can also write the extended set of equations

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t}=\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\mathbf{r}\\ \mathbf{p}\\ E_{\mathrm{int}}\end{pmatrix}=\begin{pmatrix}\frac{\partial E_{\mathrm{tot}}}{\partial \mathbf{p}}\\ -\frac{\partial E_{\mathrm{tot}}}{\partial \mathbf{r}}-\frac{\xi}{m}\mathbf{p}\\ \frac{\xi}{m^2}\mathbf{p}^2\end{pmatrix}=\underbrace{\begin{pmatrix}\mathbf{0} & \mathbf{1} & \mathbf{0}\\ -\mathbf{1} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & 0\end{pmatrix}}_{\boldsymbol{L}}\begin{pmatrix}\frac{\partial E_{\mathrm{tot}}}{\partial \mathbf{r}}\\ \frac{\partial E_{\mathrm{tot}}}{\partial \mathbf{p}}\\ 1\end{pmatrix}+\begin{pmatrix}\mathbf{0}\\ -\frac{\xi}{m}\mathbf{p}\\ \frac{\xi}{m^2}\mathbf{p}^2\end{pmatrix}$$
$$=\boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}}+\begin{pmatrix}\mathbf{0}\\ -\frac{\xi}{m}\mathbf{p}\\ \frac{\xi}{m^2}\mathbf{p}^2\end{pmatrix} \tag{2.25}$$

in some analogously geometric (differential geometric), gradient-based, form as the nonextended counterpart (2.20). This can be done in a somewhat implicit way:

$$\begin{pmatrix}\mathbf{0}\\ -\frac{\xi}{m}\mathbf{p}\\ \frac{\xi}{m^2}\mathbf{p}^2\end{pmatrix}=\frac{\mathrm{d}\Xi}{\mathrm{d}\boldsymbol{x}^*}\big(\boldsymbol{x}^*=\tfrac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}\big) \tag{2.26}$$

with

$$\Xi\left(\boldsymbol{x}^*\right)=\frac{1}{2}\left(\boldsymbol{x}^*\right)^{\mathrm{transp}}\underbrace{\begin{pmatrix}\mathbf{0} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \xi\mathbf{1} & -\frac{\xi}{m}\mathbf{p}\\ \mathbf{0} & -\frac{\xi}{m}\mathbf{p} & \frac{\xi}{m}\mathbf{p}^2\end{pmatrix}}_{\boldsymbol{M}}\boldsymbol{x}^*,\qquad \frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}=\begin{pmatrix}\mathbf{0}\\ \mathbf{0}\\ 1\end{pmatrix} \tag{2.27}$$

so a new auxiliary variable (namely, $\boldsymbol{x}^*$) has to be involved, and the matrix $\boldsymbol{M}$ that is the heart of the quadratic form Ξ is not constant but state dependent. Actually, although

$$\Xi\left(\tfrac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}\right)=mD=\frac{\xi}{2m^2}\mathbf{p}^2 \tag{2.28}$$

as expected, the gradient has to be taken with respect to the auxiliary variable ($\boldsymbol{x}^*$).

Here, for later purposes, it is useful to observe that the extended set of equations

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t}=\boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}}+\frac{\mathrm{d}\Xi}{\mathrm{d}\boldsymbol{x}^*}\big(\boldsymbol{x}^*=\tfrac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}\big) \tag{2.29}$$

can also be presented as

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t}=\boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}}+\boldsymbol{M}\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}. \tag{2.30}$$

2.6. A *constant* (state-independent) matrix $\boldsymbol{M}$ and a *simpler* setup can be achieved if we rearrange the setup in such a way that our extended set of state variables is

$$\boldsymbol{x}=\begin{pmatrix}\mathbf{r}\\ \mathbf{p}\\ E_{\mathrm{tot}}\end{pmatrix} \tag{2.31}$$

and the relationship among the various energies (the constitutive relationship) is expressed as

$$E_{\mathrm{int}}(\boldsymbol{x}) = E_{\mathrm{tot}} - K(\mathbf{p}) - U(\mathbf{r}), \tag{2.32}$$

also implying

$$\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}} = \begin{pmatrix} \frac{\partial E_{\mathrm{int}}}{\partial \mathbf{r}} \\ \frac{\partial E_{\mathrm{int}}}{\partial \mathbf{p}} \\ \frac{\partial E_{\mathrm{int}}}{\partial E_{\mathrm{tot}}} \end{pmatrix} = \begin{pmatrix} -\frac{\partial U}{\partial \mathbf{r}} \\ -\frac{\partial K}{\partial \mathbf{p}} \\ 1 \end{pmatrix} = \begin{pmatrix} -\frac{\partial U}{\partial \mathbf{r}} \\ -\frac{1}{m}\mathbf{p} \\ 1 \end{pmatrix}. \tag{2.33}$$

In this variant, a simpler set of equations has to be realized:

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \mathbf{r} \\ \mathbf{p} \\ E_{\mathrm{tot}} \end{pmatrix} = \begin{pmatrix} -\frac{\partial E_{\mathrm{int}}}{\partial \mathbf{p}} \\ \frac{\partial E_{\mathrm{int}}}{\partial \mathbf{r}} - \frac{\xi}{m}\mathbf{p} \\ 0 \end{pmatrix} = \underbrace{\begin{pmatrix} \mathbf{0} & -\mathbf{1} & \mathbf{0} \\ \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 0 \end{pmatrix}}_{\boldsymbol{L}} \begin{pmatrix} \frac{\partial E_{\mathrm{int}}}{\partial \mathbf{r}} \\ \frac{\partial E_{\mathrm{int}}}{\partial \mathbf{p}} \\ 1 \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ -\frac{\xi}{m}\mathbf{p} \\ 0 \end{pmatrix} \\ = \boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}} + \begin{pmatrix} \mathbf{0} \\ -\frac{\xi}{m}\mathbf{p} \\ 0 \end{pmatrix}; \end{aligned} \tag{2.34}$$

therefore, a simpler counterpart of (2.26) emerges, with a constant matrix $\boldsymbol{M}$:

$$\begin{pmatrix} \mathbf{0} \\ -\frac{\xi}{m}\mathbf{p} \\ 0 \end{pmatrix} = \frac{\mathrm{d}\Xi}{\mathrm{d}\boldsymbol{x}^*}\left(\boldsymbol{x}^* = \tfrac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}\right) \qquad \text{with} \qquad \Xi\left(\boldsymbol{x}^*\right) = \tfrac{1}{2}\left(\boldsymbol{x}^*\right)^{\mathrm{transp}} \underbrace{\begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \frac{\xi}{m}\mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 0 \end{pmatrix}}_{\boldsymbol{M}} \boldsymbol{x}^*. \tag{2.35}$$

We still have

$$\Xi\left(\tfrac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}\right) = mD = \tfrac{\xi}{2m^2}\mathbf{p}^2, \tag{2.36}$$

and the set of equations

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}} + \frac{\mathrm{d}\Xi}{\mathrm{d}\boldsymbol{x}^*}\left(\boldsymbol{x}^* = \tfrac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}\right) \tag{2.37}$$

also has a simpler equivalent:

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}} + \boldsymbol{M}\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}. \tag{2.38}$$

2.7. Actually, our special system admits an exceptionally direct special realization as well:

$$\begin{pmatrix} \mathbf{0} \\ -\frac{\xi}{m}\mathbf{p} \\ 0 \end{pmatrix} = -\frac{\mathrm{d}\Xi}{\mathrm{d}\boldsymbol{x}} \qquad \text{with} \qquad \Xi(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^{\mathrm{transp}} \underbrace{\begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \frac{\xi}{m^2}\mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 0 \end{pmatrix}}_{\boldsymbol{M}} \boldsymbol{x} = mD = \frac{\xi}{2m^2}\mathbf{p}^2, \tag{2.39}$$

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}} - \frac{\mathrm{d}\Xi}{\mathrm{d}\boldsymbol{x}}, \qquad \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}} - \boldsymbol{M}\boldsymbol{x}. \tag{2.40}$$

Such an extraordinarily simple formulation is not available for most other dissipative systems.

In fact, damping proportional to velocity is a distinguished case that permits a number of other special treatments as well, including [19, 20] (via a time-dependent Hamiltonian), [21] (a family generalizing the former one including a time-independent, logarithmic, realization), [22, 23] (doubling the degrees of freedom to obtain a time-independent Lagrangian–Hamiltonian–variational formulation), and [24] (adding infinitely many degrees of freedom of harmonic oscillators). On one hand, these many possibilities may indicate that this special model can emerge from rather different physical reasons. On the other hand, these realizations are not robust – even minor generalizations of this model may exclude these peculiar possibilities, and the versions like [22–24] also require fine-tuned initial conditions on the additional degrees of freedom, possibly violating time-translation invariance (which the equation of motion itself possesses). Furthermore, most of these approaches try to minimize what we know about the additional means of energy storing while in most concrete situations thermodynamics does have specific knowledge about them, and the complete model is richer than the damped mechanical part itself. Altogether, for general irreversible situations one needs more robust description.

2.8. The form seen in (2.38) is also special in a sense [compare it to (2.30)]: both matrices act on $\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}}$ (so actually we can add $\boldsymbol{L}$ and $\boldsymbol{M}$) – this is typically called a one-generator formalism (the same only E_{int} is used in the two terms). Nevertheless, such a one-generator form can be established for most known dissipative systems [25]. What needs to be generalized, both in (2.38) and (2.30), is that, for dissipative systems in general, internal energy does not increase monotonously – it is a further constitutive function, entropy (more precisely, total entropy S_{tot}) that increases monotonously. Accordingly, the general form of the set of equations is[2]

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}} + \frac{\mathrm{d}\Xi}{\mathrm{d}\boldsymbol{x}^*}\big(\boldsymbol{x}^* = \tfrac{\mathrm{d}S_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}}\big), \qquad \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}} + \boldsymbol{M}\frac{\mathrm{d}S_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}}. \tag{2.41}$$

This is the formulation known by the acronym GENERIC [6–10]. The general standard requirements on the GENERIC form [8],

$$\boldsymbol{L}^{\mathrm{transp}} = -\boldsymbol{L} \qquad \text{(antisymmetricity of } \boldsymbol{L}\text{)}, \tag{2.42}$$

$$\boldsymbol{M}^{\mathrm{transp}} = \boldsymbol{M} \qquad \text{(symmetricity of } \boldsymbol{M}\text{)}, \tag{2.43}$$

$$\boldsymbol{L}\frac{\mathrm{d}S_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}} = \boldsymbol{0}, \qquad \boldsymbol{M}\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}} = \boldsymbol{0} \qquad \text{(transversality conditions)}, \tag{2.44}$$

$$\sum_l \left(L_{il}\frac{\partial L_{jk}}{\partial x_l} + L_{jl}\frac{\partial L_{ki}}{\partial x_l} + L_{kl}\frac{\partial L_{ij}}{\partial x_l} \right) = 0 \qquad \text{(Jacobi identity for } \boldsymbol{L}\text{)} \tag{2.45}$$

ensure that

- E_{tot} is constant along any process allowed by (2.41),

[2]The second form looks a bit more general than the former but can be incorporated in the former via allowing $\Xi = \Xi(\boldsymbol{x}, \boldsymbol{x}^*)$.

- S_{tot} increases along any process allowed by (2.41) except for equilibrium solutions (the stationary – time-independent – ones),
- the reversible part induces time evolution that preserves the $\boldsymbol{L}$-induced Poisson bracket as it happens for Hamiltonian systems (see more on this in [8]).

3. Temporal thermodynamics – the modern dynamical approach to thermodynamical processes

GENERIC is a powerful formalism to realize continuum systems but is also valuable for systems with finite degrees of freedom (in other words: for systems with a finite-dimensional state space). It is a natural framework for any irreversible dynamics – in other words, for thermodynamics, where thermodynamics is understood in the modern sense. To better understand the significance of GENERIC, it is useful to overview the development of modern thermodynamics.

Historically, thermodynamics focused on temperature and its relationship to other state-parametrizing quantities (pressure, density etc.), and on energy changes (heat and work) related to changes in temperature and the other state-describing quantities. The relationships among the state-parametrizing quantities were measured under static circumstances or by waiting long enough to reach practically static circumstances, on thermodynamical bodies within which quantities (already) had a homogeneous distribution. Changes were also investigated in the quasi-static regime (always waiting long enough to reach a new static state). Accordingly, time was made irrelevant, and speeds and change rates were out of scope – with the consequence that the dependence of state-describing quantities on speeds and change rates was impossible to observe. In parallel, finitely many spatially homogenized thermodynamical bodies were considered[3], which is the lumped-parameter picture. With speeds neglected, realizing the balance of momentum was impossible, kinetic energy was also lost, and the focus was on the balance of energy, which became simplified to the balance of internal energy: the change of internal energy E_{int} was related to heat-type energy transfer and to mechanical work: in infinitesimal form,

$$\mathrm{d}E_{\mathrm{int}} = đQ + đW. \tag{3.1}$$

This was the first formulation of the First Law of Thermodynamics. Mechanical work could be expressed as

$$đW = -p\,\mathrm{d}V \tag{3.2}$$

with pressure p and volume V, but there was no means of telling *why* – due to what interactions with other thermodynamical bodies – and *how* – at what change rate – V changes. Moreover, for heat only an inequality was available:

$$đQ \geq T\,\mathrm{d}S \tag{3.3}$$

[3]As a special example, the environment is a thermodynamical body whose extensive quantities – the ones proportional to extent, *e.g.,* mass, volume, internal energy – can change due to interactions with the other thermodynamical bodies, but these changes are relatively negligible for the "large" body so its intensive quantities – those governing interaction, *e.g.,* temperature, pressure – are considered constant.

with absolute temperature T and entropy S, equality for reversible cases and strict inequality for irreversible ones. This setup was not able to reveal what process results from some given interactions plus some initial conditions on the state-describing quantities.

Later in the history of thermodynamics, the role of time became gradually recognized. Onsager's activity (irreversible interactions inducing time dependence of quantities), ideas by Fényes [26, 27] and Gyarmati [28, 29], so-called finite-time thermodynamics [30] (recognizing that there is no infinite time for changes), the endoreversible picture of thermodynamics [31] (that reversibility holds within a thermodynamical body but irreversible interactions occur at the boundaries), and Matolcsi's ordinary thermodynamics [32] (where a closed set of ordinary differential equations holds for the process in time, the equations consisting of the interactions given as state-dependent functions) led to a dynamical picture of thermodynamics. Regarding space dependence of the quantities, the lumped-parameter description may be kept – *i.e.,* with piecewise homogenized quantities –, nevertheless, irreversibility generated inside a thermodynamical body is also possible to describe [33], thus providing models for viscosity, non-Newtonian fluids, viscoelasticity of solids including the Poynting–Thomson–Zener and Kluitenberg–Verhás model families, and plasticity [33].

In this description, called *temporal thermodynamics* hereafter, the First Law of Thermodynamics (3.1) is rewritten: to an infinitesimal change in the state space, an infinitesimal time interval $\mathrm{d}t$ corresponds, we consider the heating *rate*

$$\overset{*}{Q} = \frac{đQ}{\mathrm{d}t}, \tag{3.4}$$

the working *rate*

$$\overset{*}{W} = \frac{đW}{\mathrm{d}t} = -p\frac{\mathrm{d}V}{\mathrm{d}t}, \tag{3.5}$$

and the time derivative of internal energy is related to these energy transfer rates:

$$\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}t} = \overset{*}{Q} + \overset{*}{W}. \tag{3.6}$$

In parallel to this balance of energy, there becomes possibility to realize the balance of momentum, which provides an equation for $\frac{\mathrm{d}V}{\mathrm{d}t}$. If there is a change in mass, m, or in some further state-describing quantity, then this change is also to be expressed via such equations on time derivatives. In the final form, we have a set of equations where $\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}t}$, $\frac{\mathrm{d}V}{\mathrm{d}t}$ *etc.* are on the left-hand side while $\overset{*}{Q}$ and everything else on the right-hand sides is given as concrete state-dependent functions, *interaction functions.*[4] For instance, for convective heat transfer between a thermodynamical body with temperature T and an environment with its ambient temperature T_{a}, $\overset{*}{Q}$ is proportional to $T - T_{\mathrm{a}}$ while for a thermal-radiation type interaction, $\overset{*}{Q}$ is proportional to $T^4 - T_{\mathrm{a}}^4$.

The interactions considered may be reversible or irreversible, and GENERIC provides a means of separating these two kinds. Moreover, in general, the reversible part cannot be formulated using a Lagrangian like in (2.8) or a Hamiltonian like in (2.10)

[4] A full example for this final form follows below.

– such examples are all systems with an odd number of degrees of freedom (with an odd-dimensional state space). Both the separation and the Poisson realization of the reversible part have benefits – both at the conceptual level and for solutions, in particular for numerical solutions. This is demonstrated below.

4. Applying GENERIC: Temporal thermodynamical modelling of a nonlinear process of a supercritical fluid enclosed by a piston

4.1. **Why supercritical? Why GENERIC?** Due to the product $-p\frac{\mathrm{d}V}{\mathrm{d}t}$ in the balance of energy (3.6) and the fact that, in general, both p and $\frac{\mathrm{d}V}{\mathrm{d}t}$ change along a process, temporal dynamics is nonlinear in general. In parallel, the dependence of p on the quantities E_{int}, V, *etc.* is nonlinear even for the simplest fluid model, ideal gas. Particularly strong is material nonlinearity slightly above the critical point (the point in the state space below which compressibility becomes negative, inducing instability for the thermodynamical body and forming the tip of the phase equilibrium curve).

A process running above the critical point in the state space has technological advantages. For example, the Generation IV type nuclear reactors (Super Critical Water Reactors, SCWR's) utilize supercritical water [34, 35], while other power cycles use supercritical CO_2 [36] or organic fluids with a low boiling point [37]. Because of practical considerations, processes may not run much above the critical point. Material nonlinearities are particularly strong just above the critical point – in the so-called Widom region –, which makes designing supercritical processes a delicate issue (see, *e.g.,* [38]). In this region, the rapidly varying material coefficients (compressibility, thermal expansion coefficient, and specific heat capacities) lead to strongly coupled mechanical–thermal effects, one of which is the "piston effect" (a thermally induced shock wave travelling at the speed of sound) [39–43], and another being heat transfer deterioration and enhancement [44–46]).

Trustworthy computations for such processes are important, in light of the technological applications. Nevertheless, many studies try to avoid incorporating the strong state dependences [39–41] because of difficulties in numerical simulations [47]. Thus, supercritical processes are a good and strongly justified area for seeking reliable numerical methods for irreversible dynamics. Having seen that GENERIC incorporates a number of essential aspects of irreversible dynamics, in what follows, we establish the GENERIC realization of a finite degree-of-freedom setup for a supercritical fluid, and then study numerical schemes for this setup that provide some insight and general lessons regarding reliability.

4.2. **The fluid considered in the supercritical regime.** The (quasi-static) thermal equation of state – also known as the thermal constitutive relationship – of a simple fluid can be given through the function $p(T, v)$ (for pressure p, temperature T, and specific volume $v = V/m$ with volume V and mass m). For definiteness, we treat here the van der Waals (vdW) model, for which

$$p(T, v) = \frac{RT}{v - \mathtt{b}} - \frac{\mathtt{a}}{v^2} \qquad (R > 0,\ \mathtt{a} > 0,\ \mathtt{b} > 0). \tag{4.1}$$

In this fluid model, the critical point (the solution of the pair of $\frac{\partial p}{\partial v}\Big|_T = 0$, $\frac{\partial^2 p}{\partial v^2}\Big|_T = 0$, see, *e.g.,* [33]) is characterized by the critical values

$$p_{\mathrm{c}} = \frac{1}{27}\frac{\mathtt{a}}{\mathtt{b}^2}, \quad T_{\mathrm{c}} = \frac{8}{27}\frac{\mathtt{a}}{R\mathtt{b}}, \quad v_{\mathrm{c}} = 3\mathtt{b}. \tag{4.2}$$

In order to ensure that the numerical computations below can work with dimensionless quantities, we introduce the dimensionless reduced quantities

$$\check{p} = \frac{p}{p_{\mathrm{c}}}, \quad \check{T} = \frac{T}{T_{\mathrm{c}}}, \quad \check{v} = \frac{v}{v_{\mathrm{c}}}, \tag{4.3}$$

via which (4.1) becomes

$$\check{p}\big(\check{T}, \check{v}\big) = \frac{8\check{T}}{3\check{v} - 1} - \frac{3}{\check{v}^2}. \tag{4.4}$$

In addition, we use the caloric constitutive relationship, with $e_{\mathrm{int}} = E_{\mathrm{int}}/m$,

$$e_{\mathrm{int}}(T, v) = \frac{\mathtt{f}}{2}RT - \frac{\mathtt{a}}{v}, \qquad \Rightarrow\ \check{e}_{\mathrm{int}} = \frac{e_{\mathrm{int}}}{p_{\mathrm{c}} v_{\mathrm{c}}} = \frac{4}{3}\mathtt{f}\check{T} - \frac{3}{\check{v}}, \tag{4.5}$$

which is consistent [33] with the thermal constitutive function (4.1) and gives, in the ideal-gas limit, the case of constant isochoric specific heat $c_v = \frac{\mathtt{f}}{2}R$; the molecular energy-storing degree of freedom $\mathtt{f}$ is set to 3 in the subsequent computations (the outcomes have proven to be qualitatively the same for other values of $\mathtt{f}$).

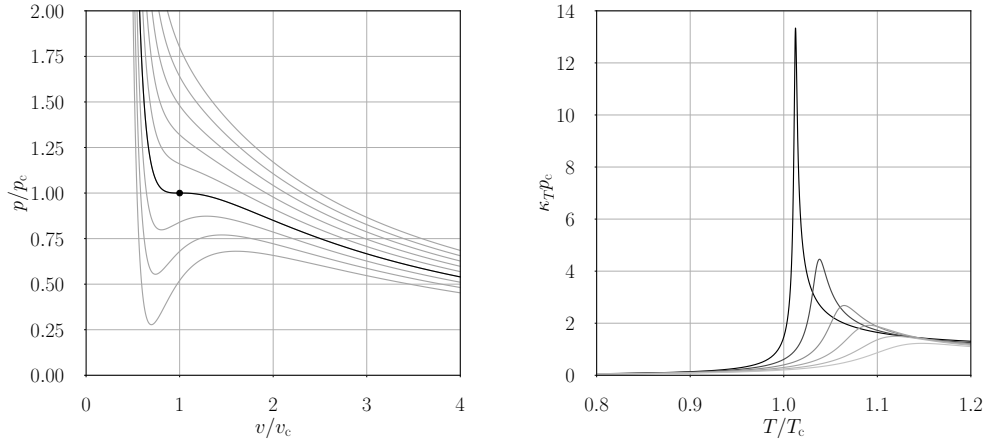


Figure 1. *Left:* isothermal lines of the van der Waals material, and the critical point. *Right*: As pressure approaches critical pressure from above, a sharper-and-sharper maximum is observable in isothermal compressibility. For isobaric thermal expansion and for isobaric specific heat capacity, a similar behaviour is observable.

In any simple fluid model, the isothermal compressibility

$$\kappa_T = -\frac{1}{v}\left.\frac{\partial v}{\partial p}\right|_T = -\frac{1}{v}\frac{1}{\left.\frac{\partial p}{\partial v}\right|_T}, \tag{4.6}$$

the isobaric volumetric thermal expansion coefficient

$$\alpha = \frac{1}{v}\left.\frac{\partial v}{\partial T}\right|_p = -\frac{1}{v}\frac{\left.\frac{\partial p}{\partial T}\right|_v}{\left.\frac{\partial p}{\partial v}\right|_T}, \tag{4.7}$$

and the isobaric specific heat capacity

$$c_p = \frac{1}{m}\frac{\text{đ}Q\big|_p}{\mathrm{d}T\big|_p} = \left.\frac{\partial e_{\text{int}}}{\partial T}\right|_p + p\left.\frac{\partial v}{\partial T}\right|_p \tag{4.8}$$

are defined [33] and prove to be very informative for a wide range of aspects. If we approach the critical point, from above (in temperature or pressure), then each of these become heavily state dependent and diverge, as illustrated in Fig. 1. The strong state dependence makes processes running near the critical point considerably nonlinear.

A closing comment regarding the constitutive relationships is that the dynamical equations below will determine e_{int} and v. Then T can be obtained through expressing it from $e_{\text{int}}(T, v)$ [in our present case, from (4.5)]. Then this $T(e_{\text{int}}, v)$ can be put into p:

$$p(T, v) \equiv p\big(T(e_{\text{int}}, v), v\big) \equiv p\left(e_{\text{int}}, v\right) \tag{4.9}$$

so p is also available as function of e_{int} and v.

4.3. **The setup considered and its dynamical equations.** The problem we study hereafter is as follows. A fixed amount of supercritical van der Waals fluid is enclosed in a cylinder, separated from the environment by a movable rigid piston (see Fig. 2). We assume adiabatic circumstances, enabling mechanical interaction only. As explained in Section 3, for a temporal, dynamical process, a closed set of ordinary differential equations is needed.

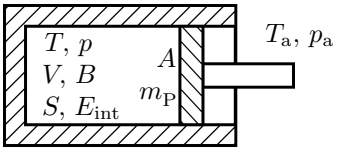


Figure 2. The setup of a supercritical fluid enclosed in a cylinder by a movable rigid piston, and the relevant quantities of the fluid, of the piston, and of the environment (subscript 'a' refers to 'ambient').

The first of these is the First Law of Thermodynamics – the balance for energy – considered as the relationship (3.6) among the change rate (time derivative) of internal

energy, heating rate and working rate (with the heating rate now actually being zero according to the adiabatic assumption).

In parallel, for the piston, we write Newton's equation of motion, which determines acceleration from the force exerted by the fluid and the force stemming from external (ambient) pressure. This is actually the balance for momentum.

Finally, the change rate of volume is to be connected to the velocity of the piston.

The details are as follows.

The intensive quantities of the large environment are not influenced by the process, so ambient temperature T_a and ambient pressure p_a are considered constant:

$$T_\mathrm{a} = \mathrm{const.}, \qquad p_\mathrm{a} = \mathrm{const.} \tag{4.10}$$

The piston is characterized by its mass m_P and the cross-section area A.

Corresponding to the step where, in mechanics, the time derivative of position is raised to the level of a physical quantity – velocity – here the time derivative of volume, $\mathrm{d}V/\,\mathrm{d}t$, is raised to the level of a quantity on its own right, denoted hereafter by B:

$$V = Ax, \quad \frac{\mathrm{d}V}{\mathrm{d}t} = A\frac{\mathrm{dx}}{\mathrm{d}t}: \quad B = Av \tag{4.11}$$

(where x is the position coordinate of the piston and v is its velocity).

Due to the rigid piston, there is a conservation rule for the involved volumes, the time derivative of which connects the ambient volume change rate B_a with the volume change rate B of the enclosed fluid:

$$V_\mathrm{a} = V_\mathrm{tot} - V, \qquad B_\mathrm{a} = -B. \tag{4.12}$$

The conserved total energy, E_tot consists of the internal energy E_int of the fluid, the kinetic energy of the piston – expressible as

$$\frac{m_\mathrm{P}}{2}\left(\frac{B}{A}\right)^2 = \frac{\chi_\mathrm{P}}{2}B^2 \qquad \text{with} \quad \chi_\mathrm{P}{=}\frac{m_\mathrm{P}}{A^2}, \tag{4.13}$$

and the ambient internal energy, from which only a term $-p_\mathrm{a}V_\mathrm{a} = p_\mathrm{a}V + \mathrm{const.}$ has time dependence, as we have neglected heat-type interaction and allowed only mechanical work-type interaction:

$$E_\mathrm{tot} = E_\mathrm{int} + \frac{\chi_\mathrm{P}}{2}B^2 + p_\mathrm{a}V + \mathrm{const.} \tag{4.14}$$

We mention that, regarding (4.14), the Appendix provides further insight.

In addition to the reversible pressure seen in (4.1), and denoted hereafter by p_rev, we also allow for an optional irreversible, dissipative, viscosity-type pressure contribution

$$p_\mathrm{irr} = -\beta b \qquad \text{with} \quad b = \frac{B}{m} \tag{4.15}$$

(where $\beta \geq 0$ may be state dependent; see, e.g., [48]), so

$$p = p_\mathrm{rev} + p_\mathrm{irr} = p_\mathrm{rev}(T, v) - \beta(T, v, b) \cdot b. \tag{4.16}$$

Then the mentioned three temporal differential equations – the First Law, the kinematic relationship, and the equation of motion of the piston – are concretized as

$$\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}t} = -pB, \tag{4.17}$$

$$\frac{\mathrm{d}V}{\mathrm{d}t} = B, \tag{4.18}$$

$$m_{\mathrm{P}}\frac{\mathrm{d}\frac{B}{A}}{\mathrm{d}t} = pA - p_{\mathrm{a}}A \quad \Longrightarrow \quad \frac{\mathrm{d}B}{\mathrm{d}t} = \frac{1}{\chi_{\mathrm{P}}}\left(p - p_{\mathrm{a}}\right), \tag{4.19}$$

they form a closed set of equations, and together ensure conservation of total energy, $\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}t} = 0$ along a process, as is straightforward to show.

Note that there is an odd number (3) of degrees of freedom here, so even the reversible case $\beta = 0$ is non-Hamiltonian and cannot have a symplectic structure.

4.4. **GENERIC formulation of the model.** The GENERIC form of our set of temporal differential equations (4.17)–(4.19) should be [see (2.41)]

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x} = \boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}} + \boldsymbol{M}\frac{\mathrm{d}S_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}}, \tag{4.20}$$

where $\boldsymbol{x}$ is a collection of state variables. For (4.17)–(4.19), $\boldsymbol{x} = \begin{pmatrix} E_{\mathrm{int}} & V & B \end{pmatrix}^{\mathrm{transp}}$, and E_{tot} is given in (4.14). Furthermore, regarding

$$S_{\mathrm{tot}} = S + S_{\mathrm{a}}, \qquad \mathrm{d}S_{\mathrm{tot}} = \mathrm{d}S + \mathrm{d}S_{\mathrm{a}}, \qquad \frac{\mathrm{d}S_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}} = \frac{\mathrm{d}S}{\mathrm{d}\boldsymbol{x}} + \frac{\mathrm{d}S_{\mathrm{a}}}{\mathrm{d}\boldsymbol{x}}, \tag{4.21}$$

the constitutive definition of entropy S gives (see, *e.g.,* [33]), for constant mass,

$$\mathrm{d}S = \frac{1}{T}\,\mathrm{d}E_{\mathrm{int}} + \frac{p_{\mathrm{rev}}}{T}\,\mathrm{d}V \qquad \Longrightarrow \qquad \frac{\mathrm{d}S}{\mathrm{d}\boldsymbol{x}} = \frac{1}{T}\frac{\mathrm{d}E_{\mathrm{int}}}{\mathrm{d}\boldsymbol{x}} + \frac{p_{\mathrm{rev}}}{T}\frac{\mathrm{d}V}{\mathrm{d}\boldsymbol{x}}, \tag{4.22}$$

while S_{a} does not depend on $\boldsymbol{x}$ as it is a constitutive function of the state variables of the environment, not of the state variables of the enclosed fluid. Then it is not difficult to check that the structure (4.20) can be realized as

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} E_{\mathrm{int}} \\ V \\ B \end{pmatrix} = \begin{pmatrix} 0 & 0 & -\frac{p_{\mathrm{rev}}}{\chi_{\mathrm{P}}} \\ 0 & 0 & \frac{1}{\chi_{\mathrm{P}}} \\ \frac{p_{\mathrm{rev}}}{\chi_{\mathrm{P}}} & -\frac{1}{\chi_{\mathrm{P}}} & 0 \end{pmatrix}\begin{pmatrix} 1 \\ p_{\mathrm{a}} \\ \chi_{\mathrm{P}}B \end{pmatrix} + \begin{pmatrix} \frac{T\beta}{m}B^2 & 0 & \frac{Tp_{\mathrm{irr}}}{\chi_{\mathrm{P}}} \\ 0 & 0 & 0 \\ \frac{Tp_{\mathrm{irr}}}{\chi_{\mathrm{P}}} & 0 & \frac{T\beta}{m\chi_{\mathrm{P}}^2} \end{pmatrix}\begin{pmatrix} \frac{1}{T} \\ \frac{p_{\mathrm{rev}}}{T} \\ 0 \end{pmatrix}, \tag{4.23}$$

where the standard requirements (2.42)–(2.45) are straightforwardly fulfilled. It is worth mentioning that, in particular,

$$\frac{\mathrm{d}S_{\mathrm{tot}}}{\mathrm{d}t} \geq 0 \qquad \text{(equality only at equilibrium)} \tag{4.24}$$

is realized as

$$\frac{\mathrm{d}S_{\mathrm{tot}}}{\mathrm{d}t} = \frac{\beta}{m}\frac{B^2}{T}, \tag{4.25}$$

i.e., the only source of irreversibility (entropy generation) is the optional irreversible pressure contribution.

In order to provide an outlook, in the Appendix, the generalization of (4.23) is presented when adiabaticity is replaced by a nonzero heating rate.

5. Symplectic numerical schemes and the quasi-symplectic extension introduced here

5.1. **The starting point: symplectic numerical schemes.** If dynamics is reversible,

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{L}\frac{\mathrm{d}E_{\mathrm{tot}}}{\mathrm{d}\boldsymbol{x}}, \tag{5.1}$$

with a nondegenerate $\boldsymbol{L}$ – this necessitates an even-dimensional state space (phase space) – and if antisymmetricity and the Jacobi property (2.45) are satisfied, then the system is *symplectic*, *i.e.,* with $\tilde{\boldsymbol{x}}\,(t, \boldsymbol{x}_0)$ denoting the solution at t for the initial condition $\boldsymbol{x}_0$ at t_0,

$$\left(\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{x}_0}\tilde{\boldsymbol{x}}\,(t, \boldsymbol{x}_0)\right)^{\mathrm{transp}} \boldsymbol{L}^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{x}_0}\tilde{\boldsymbol{x}}\,(t, \boldsymbol{x}_0)\right) = \boldsymbol{L}^{-1}, \tag{5.2}$$

in other words, the left-hand side of (5.2) is t-independent.

In such cases, via variable transformation, $\boldsymbol{x}$ can be transformed to a half-split (partitioned) form

$$\boldsymbol{x} = \begin{pmatrix}\mathbf{q}\\ \mathbf{p}\end{pmatrix} \tag{5.3}$$

(both $\mathbf{q}$ and $\mathbf{p}$ being half as many degrees of freedom as $\boldsymbol{x}$) in which the dynamical equations become simplified to

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{p}}, \qquad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \mathbf{q}}, \tag{5.4}$$

where the Hamiltonian $H(\mathbf{q}, \mathbf{p})$ is the transformed form of $E_{\mathrm{tot}}(\boldsymbol{x})$. Equations (5.3) are generalized version of (2.10).

Let us now turn toward numerical, finite-difference solutions of (5.4). An equidistant temporal discretization is considered: in notation, the discrete time instants are $t^j = j\cdot\Delta t,\ j = 0, 1, \ldots, J$, where Δt is the size of the chosen time step. The value of a function in the jth time instant is denoted by a superscript j, for example, $\mathbf{q}\big(t^j\big) = \mathbf{q}^j$. Time derivatives are discretized as ratios of differences, for instance, $\frac{\mathbf{q}^{j+1}-\mathbf{q}^j}{\Delta t}$.

A first-order numerical method is the explicit Euler scheme, which for (5.4) reads

$$\mathbf{q}^{j+1} = \mathbf{q}^j + \Delta t\frac{\partial H}{\partial \mathbf{p}}\left(\mathbf{q}^j, \mathbf{p}^j\right), \qquad \mathbf{p}^{j+1} = \mathbf{p}^j - \Delta t\frac{\partial H}{\partial \mathbf{q}}\left(\mathbf{q}^j, \mathbf{p}^j\right). \tag{5.5}$$

Its variants, the also first-order but much better performing two versions of the so-called symplectic Euler scheme

$$\mathbf{q}^{j+1} = \mathbf{q}^j + \Delta t\frac{\partial H}{\partial \mathbf{p}}\left(\mathbf{q}^j, \mathbf{p}^{j+1}\right), \qquad \mathbf{p}^{j+1} = \mathbf{p}^j - \Delta t\frac{\partial H}{\partial \mathbf{q}}\left(\mathbf{q}^j, \mathbf{p}^{j+1}\right) \tag{5.6}$$

and

$$\mathbf{q}^{j+1} = \mathbf{q}^j + \Delta t \frac{\partial H}{\partial \mathbf{p}}\left(\mathbf{q}^{j+1}, \mathbf{p}^j\right), \qquad \mathbf{p}^{j+1} = \mathbf{p}^j - \Delta t \frac{\partial H}{\partial \mathbf{q}}\left(\mathbf{q}^{j+1}, \mathbf{p}^j\right), \tag{5.7}$$

are examples of symplectic numerical methods (see, *e.g.,* [3, 49]). Symplectic schemes preserve the symplectic structure [see (5.2)], and actually provide the *exact* solution of a nearby Hamiltonian system. This is the background behind their good performance. Other examples of symplectic methods are the Störmer–Verlet scheme (giving the leapfrog method for special cases) and the symplectic Runge–Kutta family.

It is worth mentioning here that Backward Error Analysis (BEA) is able to find the distorted (the nearby) Hamiltonian, to any desired order of Δt. Then compensations can be introduced to improve the performance of the given scheme. This is the technique used in [1] to improve the second-order Newmark method to fourth-order accuracy.

For irreversible systems, the situation is much more difficult but a systematic suggestion to make use of the properties of the symplectic methods and of BEA within GENERIC was made in [14]. This is one way GENERIC can be helpful in this respect. Besides this, at a more general level, GENERIC encourages us to make symplectic schemes "survive" for irreversible systems, in the hope that the benefits are at least partially inherited to the irreversible level.

Accordingly, here, we separate our variables into two groups, to mimic (5.3), and to generalize the symplectic Euler scheme (5.7). The details are as follows.

5.2. **The quasi-symplectic scheme.** We work with dimensionless quantities defined via the units as already introduced in (4.3) while, for time-related quantities, χ_{P} is used as the fourth necessary unit.

Our separation of the degrees of freedom is such that $\check{v}$ and $\check{e}_{\mathrm{int}}$ are the "generalized **q**-type" quantities and $\check{b}$ is the "generalized **p**-type" [cf. (5.3)], and our discretization corresponding to (4.17)–(4.19) is

$$\check{v}^{j+1} = \check{v}^j + \Delta\check{t}\check{b}^j, \tag{5.8}$$

$$\check{e}_{\mathrm{int}}^{j+1} = \check{e}_{\mathrm{int}}^{j} - \Delta\check{t}\check{p}^j\check{b}^j, \tag{5.9}$$

$$\check{T}^{j+1} = \frac{3}{4\mathtt{f}}\left(\check{e}_{\mathrm{int}}^{j+1} + \frac{3}{\check{v}^{j+1}}\right), \tag{5.10}$$

$$\check{p}_{\mathrm{rev}}^{j+1} = \frac{8\check{T}^{j+1}}{3\check{v}^{j+1} - 1} - \frac{3}{\left(\check{v}^{j+1}\right)^2}, \tag{5.11}$$

$$\check{p}_{\mathrm{irr}}^{j+1} = -\check{\beta}\left[\left(1-\alpha_p\right)\check{b}^j + \alpha_p\check{b}^{j+1}\right], \tag{5.12}$$

$$\check{b}^{j+1} = \check{b}^j + \Delta\check{t}\left[\left(1-\alpha_b\right)\left(\check{p}_{\mathrm{rev}}^{j} + \check{p}_{\mathrm{irr}}^{j}\right) + \alpha_b\left(\check{p}_{\mathrm{rev}}^{j+1} + \check{p}_{\mathrm{irr}}^{j+1}\right) - \check{p}_{\mathrm{a}}\right], \tag{5.13}$$

$$\check{p}^{j+1} = \check{p}^{j+1}_{\mathrm{rev}} + \check{p}^{j+1}_{\mathrm{irr}} \tag{5.14}$$

where α_p and α_b are arbitrary constants between 0 and 1, with which the implicitness of the scheme can be controlled. More closely:

- When the process is reversible, *i.e.,* $\check{\beta} = 0$, then $\alpha_b = 0$ realizes the explicit Euler method, while $\alpha_b = 1$ results in a quasi-symplectic – generalized symplectic Euler – scheme.
- The case when dissipation is also included, *i.e.,* $\check{\beta} > 0$, carries some additional richness. Namely, since equation (5.12) is the discrete version of a constitutive equation – an algebraic one, (4.15) – then the natural choice is $\alpha_p = 1$. In this case $\alpha_b = 0$ still represents the explicit Euler method while $\alpha_b = 1$ is a thermodynamically extended quasi-symplectic method, where the scheme becomes implicit (namely, (5.12) and (5.13) need to be solved as a coupled pair of equations).

Our aim with the optional viscosity-like damping is twofold. First, in practical applications, it may represent a reasonable model for mechanical losses [48]. Second, even if there is no irreversible pressure contribution in the problem itself, $\check{p}_{\mathrm{irr}}$ can realize artificial viscosity, which is a typical practice in simulations to counterbalance numerical artifacts. In Subsection 6.2 we show such a study for this technique.

For simplicity, when $\check{\beta} > 0$, we consider a constant $\check{\beta}$.

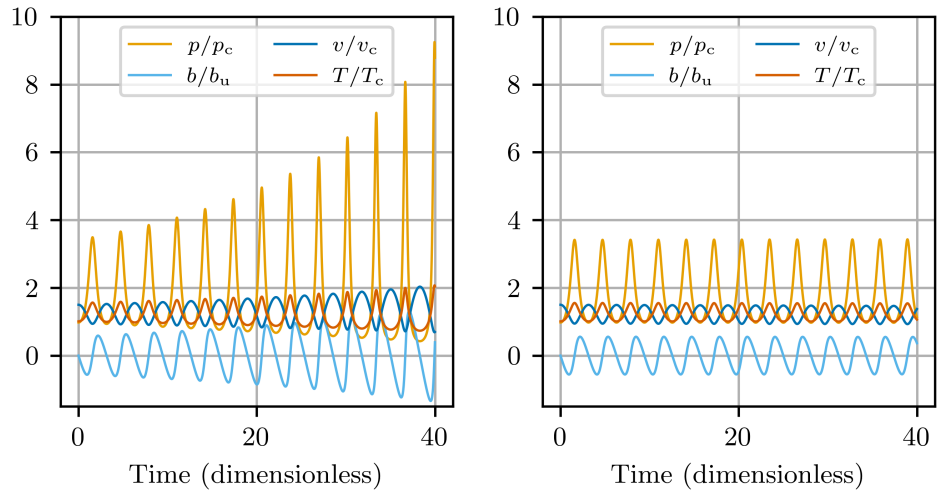
Despite the fact that our problem is an odd-dimensional system and symplectic methods are developed for even-dimensional ones, and despite possibly having an irreversible rather than reversible system, the symplectic starting point yields a better-performing numerical method than the corresponding traditional one, as shown in the following section.

6. Numerical results

6.1. **No damping: explicit Euler vs. quasi-symplectic.** First, the performance of the different numerical schemes is investigated when there is no damping in the system, *i.e.,* $\check{\beta} = 0$. As seen above, then the schemes do not depend on the parameter α_p. The initial conditions used are

$$\check{v}(0) = 1.5, \quad \check{T}(0) = 1.01, \quad \check{b}(0) = 0, \tag{6.1}$$

to which $\check{p}(0) = 0.9752$ corresponds. Furthermore, $\check{p}_{\mathrm{a}} = 1.8$ is applied. These values are chosen in such a way that the process will cross the Widom line corresponding to κ_T during oscillation (as will be demonstrated in Fig. 4 below) so that the effect of the suddenly changing compressibility can heavily influence the trajectory of the system. The initial conditions for $\check{p}(0)$ and $\check{e}_{\mathrm{int}}(0)$ are computed using the constitutive relations (4.4) and (4.5b).



(a) Result from the explicit Euler scheme. (b) Result from the quasi-symplectic scheme.

Figure 3. (a) The explicit Euler numerical scheme ($\alpha_b = 0$) provides an unacceptable solution, with artificially increasing amplitudes. (b) The quasi-symplectic enhancement of the scheme ($\alpha_b = 1$) yields a much more acceptable outcome, keeping amplitudes approximately constant. (Computations performed with $\Delta\check{t} = 0.001$.)

Fig. 3a shows the result of a simulation with $\alpha_b = 0$ (the classic explicit Euler scheme) using time step $\Delta\check{t} = 0.001$ until $\check{t}_{\mathrm{end}} = 40$. It is apparent that, due to the nonlinearity of the problem, the explicit Euler method is unable to accurately reproduce the system behaviour with these parameters, as the closed and undamped system should oscillate at a constant amplitude. The energy- and, here, amplitude-increasing effect of the explicit Euler scheme is well known [3], but in this case, it is even more pronounced due to the nature of the problem. One could instead use higher-order or implicit schemes such as the 4th-order Runge–Kutta scheme or the implicit midpoint method, or use finer time steps, but all these need increased computing resources. We demonstrate that a more appropriate scheme does not require such measures.

The reliable and satisfactorily accurate quasi-symplectic simulation enables us to examine the nonlinear oscillations in greater depth. Fig. 4 shows, using the results of the quasi-symplectic simulation, that the process indeed crosses the κ_T Widom line.

Namely, if $\alpha_b = 1$ (yielding our quasi-symplectic scheme) then the method is still first-order accurate and the scheme is still explicit, but the results are significantly more reliable. This is visible in Fig. 3b, where the amplitude of the oscillations is approximately constant during the simulation time. It is worth emphasizing here again that the only difference between the two schemes is whether $\check{p}^j$ or $\check{p}^{j+1}$ is used

for computing b^{j+1}. The change in accuracy can be attributed to the symplectic-originated symplectic-Euler nature of the quasi-symplectic scheme. This approach is similar, but not identical, to that introduced and applied in [15, 16, 50] for wave propagation with irreversible – non-Newtonian – damping.

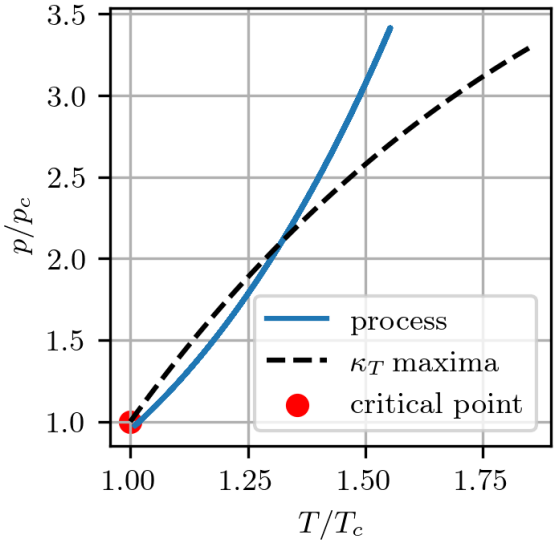
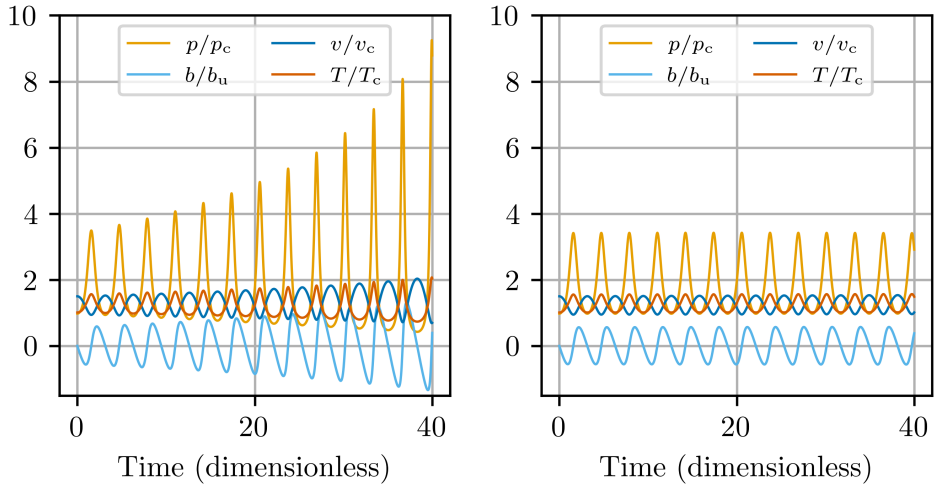


Figure 4. Trajectory of the process in the supercritical region, starting from the vicinity of the critical point, and crossing the κ_T Widom line (the collection of isobaric maxima of κ_T in the state space)

6.2. **Explicit Euler: without and with artificial damping.** As presented above, when dissipation is not taken into consideration, the system exhibits undamped oscillations. In contrast to this, when $\check{\beta} > 0$, the system is expected to tend towards an equilibrium solution, with the oscillating quantities having decreasing amplitudes.

Let us now consider the explicit Euler scheme, along with one application of nonzero dissipation.

As we have already mentioned, the dissipation may be part of the physical system or may be introduced in the numerical scheme for the role of artificial dissipation, which may compensate for artificial tendencies in the numerical solution. As seen in Fig. 3a, the explicit Euler scheme makes a nondissipative system "antidissipative". The increase of the amplitudes could be "tamed" by switching on some amount of dissipation – with an appropriate value of the damping coefficient $\check{\beta}$, the amount of artificial dissipation may render the amplitudes approximately constant. Fig. 5 shows that this can in fact be carried out.



(a) Explicit Euler solution, no damping ($\check{\beta} = 0$).

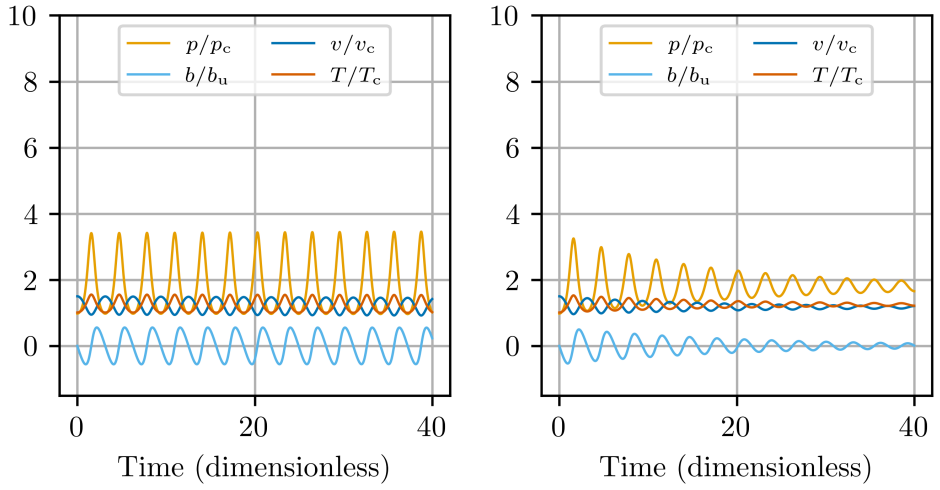
(b) Explicit Euler solution with damping $\check{\beta} = 0.04$.

Figure 5. The gradually exploding oscillations produced by the explicit Euler numerical scheme for a nondissipative system (a) can be corrected to approximately constant amplitudes (b) via a suitable amount of artificial dissipation added. ($\alpha_b = 0$, $\alpha_p = 0$, $\Delta\check{t} = 0.01$).

We mention, nevertheless, that this technique of artificial damping is not yet an automatically performable one: it is not some general algorithm that determines the optimal value of the artificial damping coefficient for a given system and given initial conditions. A compensation method to counterweigh the scheme-induced damping has recently been worked out for linear differential equations [1] so a nonlinear generalization of this approach may, in the future, provide such an algorithm.

6.3. **Quasi-symplectic: without and with damping.** With such an alternative, a much more reliable quasi-symplectic variant ($\alpha_b = 1$, $\alpha_p = 1$ in our above scheme), one can study real, physical, dissipation satisfactorily. Fig. 6 compares a solution for the nondissipative system with that for a dissipative one. Amplitudes are approximately constant in Fig. 6a and decrease in Fig. 6b as they should.

6.4. **Studying nonlinearity.** As already mentioned above, the remarkable state dependence of the thermophysical parameters makes oscillations considerably nonlinear. Fig. 3b already displays that the oscillations themselves are nonlinear, *i.e.,* nonsinusoidal, tilted, and distorted; nevertheless, we would also like to *quantify* the extent of nonlinearity.



(a) Quasi-symplectic solution, no damping ($\check{\beta} = 0$).

(b) Quasi-symplectic solution for damping $\check{\beta} = 0.1$.

Figure 6. Nondissipative (a) and dissipative (b) oscillations computed via the implicit quasi-symplectic scheme ($\alpha_b = 1$, $\alpha_p = 1$, $\Delta\check{t} = 0.01$).

If we had harmonic oscillations, then, due to the structure of the governing equation of an undamped linear (harmonic) oscillator

$$\ddot{v} = -\omega^2 (v - v_{\text{eq}}) = -\omega^2 v + \text{const.} \tag{6.2}$$

(overdot abbreviating time derivative), the trajectory of the process would be a straight line in the plane $\ddot{v}$–v. Deviation from this straight line characterizes nonlinearness . To quantify this, we introduce a measure of nonlinearity, in the form

$$\zeta = \frac{\max_j \left|\ddot{\check{v}}^j - \left(\bar{A}\check{v}^j + \bar{B}\right)\right|}{\max_j \ddot{\check{v}}^j - \min_j \ddot{\check{v}}^j}, \tag{6.3}$$

where $\bar{A}$ and $\bar{B}$ realize the straight-line trajectory of the corresponding harmonic oscillator between the two given endpoints:

$$\bar{A} = \frac{\ddot{\check{v}}\left(\check{v}_{\max}\right) - \ddot{\check{v}}\left(\check{v}_{\min}\right)}{\check{v}_{\max} - \check{v}_{\min}}, \qquad \bar{B} = \ddot{\check{v}}\left(\check{v}_{\min}\right) - \bar{A}\check{v}_{\min} \tag{6.4}$$

with the endpoint values of $\check{v}$,

$$\check{v}_{\min} = \min_j \check{v}^j, \qquad \check{v}_{\max} = \max_j \check{v}^j, \tag{6.5}$$

and $\ddot{\check{v}}\left(\check{v}_{\min}\right)$, $\ddot{\check{v}}\left(\check{v}_{\max}\right)$ being the two endpoint values of $\ddot{\check{v}}$. The measure ζ is dimensionless, equals 0 for a linear oscillation, and increases with the maximal vertical deviation from the linear trajectory. Emerging non-linear behavior near the critical point is illustrated via Figure 7.

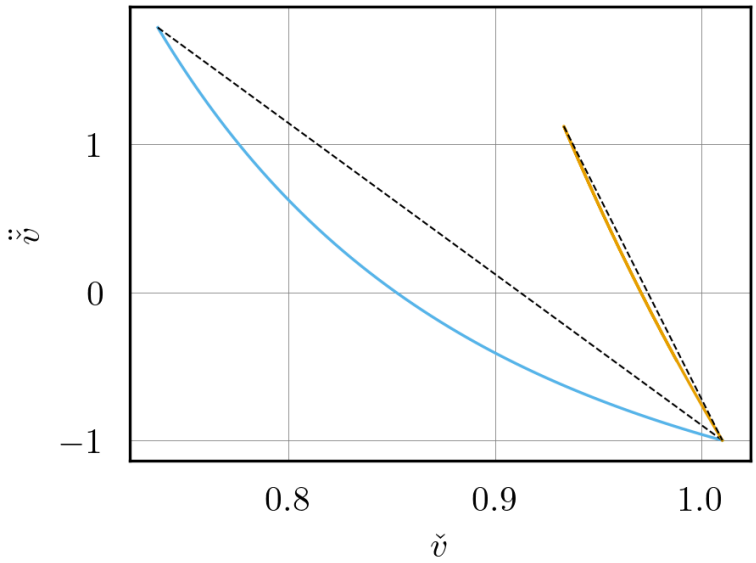


Figure 7. Nonlinearity of the resulting oscillations demonstrated. Orange: approximately linear oscillation ($\zeta = 0.0434$) far from the critical point, with initial conditions $\check{T}(0) = 3.0$, $\check{v}(0) = 1.01$, $\Rightarrow$ $\check{p}(0) = 8.8818$. Blue: nonlinear oscillation ($\zeta = 0.2195$) near the critical point, with initial conditions $\check{T}(0) = 0.999$, $\check{v}(0) = 1.01$, $\Rightarrow$ $\check{p}(0) = 0.9960$. In order to ensure a fair comparison, in both cases, $\check{p}_\mathrm{a} = \check{p}(0) + 1$. The gray dashed lines illustrate the trajectories of the corresponding linear oscillators.

Unlike other, already known, measures for nonlinearity (see, e.g., [51–53]), our new measure defined by (6.3) does not require the data to be described by a function (which, for some existing measures, also needs to be continuous or even differentiable). This property makes it applicable for datasets from simulations. Naturally, if needed, some smoothing of the data is possible. Furthermore, our measure respects the differing dimensionality of the two axes while being nondimensional itself. (Note that there is no "orthogonal" distance in a plane of dimensionally differing axes.)

7. Discussion

The quasi-symplectic Euler scheme introduced here performed considerably better than the explicit Euler one, although both are first-order methods. As such, it was possible to compute a process crossing the Widom line in the very sensitive supercritical domain much more reliably. Among other aspects, dissipation was treated

much more properly. This enabled us to investigate a deliberately introduced artificial viscosity, for which further study is needed to automatize computation of the corresponding artificial viscosity coefficient.

In order to characterize the nonlinearity of processes, both a visualization and an informative and quantitative measure that is easily determinable numerically were defined and illustrated. These demonstrated that processes in the vicinity of the critical point are remarkably nonlinear.

As a future step, higher-order symplectic methods like the Störmer–Verlet method could also be generalized to the present test problem. In the Störmer–Verlet case, for example, not only the higher order is expected to help but the balance-friendly nature of the Störmer–Verlet (leapfrog) structure also, which was already observed in [15–18].

The nonadiabatic generalization of our setup – detailed in the Appendix – offers further possibilities for future investigations. Connected to this additional source of irreversibility, more could be learned about devising optimal artificial damping.

GENERIC – the framework in which both the investigated system and its nonadiabatic counterpart have been realized here – is a motivating force for establishing numerical schemes for irreversible dynamical systems that are symplectic methods for reversible Hamiltonian special cases. Furthermore, research along the lines of [14] is expected to lead to better structure-preserving schemes for irreversible dynamical systems, preserving both the GENERIC structure and the underlying balances.

The entropy-based version of the GENERIC dynamical equations constructed here promises extra good performance for these schemes since the revealed operator content is more robust against numerical error due to the fact that the reversible operator is state-independent. This also carries the general message that thermodynamically appropriate variables and thermodynamically appropriate discretizations may be beneficial, since a considerable part of the strong thermodynamical structure can be preserved during discretization.

Author contributions. T. Fülöp: the Rayleigh case, GENERIC equations for the piston problem, conceptual aspects regarding the numerical schemes, supervision, manuscript text. M. Szücs: contribution to the Rayleigh case, numerical computations for damping and for nonlinearity, manuscript text. D. M. Takács: quasi-symplectic numerical scheme vs. explicit Euler scheme, conceptual idea for artificial damping, measure of nonlinearity, visualization method for nonlinearity, manuscript text.

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Appendix A. With heat transfer through the piston

Here, we present the generalization of (4.23) when, in addition to the mechanical interaction with the environment with working rate $\overset{*}{W} \equiv \frac{đW}{dt} = -p\frac{dV}{dt} = -pB$, adiabaticity [see (4.17)] is replaced by a nonzero heating rate $\overset{*}{Q} \equiv \frac{đQ}{dt}$. Then an additional state variable becomes necessary for the description of the dynamics. A good choice for this is S_a, which proves to be constant in the adiabatic case but becomes time-dependent for a nonzero heating rate:

$$\frac{dS_a}{dt} = \frac{\overset{*}{Q}_a}{T_a} = -\frac{\overset{*}{Q}}{T_a} \tag{A.1}$$

since, for heat transfer interaction functions in general [*e.g.,* convective $\overset{*}{Q} \sim (T - T_a)$ or radiative $\overset{*}{Q} \sim \left(T^4 - T_a^4\right)$], $\overset{*}{Q}_a = -\overset{*}{Q}$ (see, *e.g.,* [33]). In parallel to that, due to Euler homogeneity, for a fluid with constant mass,

$$E_{int} = TS - pV + \text{const.} \tag{A.2}$$

(see, *e.g.,* [33]), for the environment

$$E_{int_a} = T_a S_a - p_a V_a + \text{const.}, \tag{A.3}$$

holds. In light of (4.12a), total energy can be written as

$$E_{tot} = E_{int} + \frac{\chi_P}{2}B^2 + p_a V + T_a S_a + \text{const.} \tag{A.4}$$

[being the generalization of (4.14b)].

The GENERIC realization for $\boldsymbol{x} = \begin{pmatrix} E_{int} & V & B & S_a \end{pmatrix}^T$ is

$$\frac{d}{dt}\begin{pmatrix} E_{int} \\ V \\ B \\ S_a \end{pmatrix} = \begin{pmatrix} 0 & 0 & -\frac{p_{rev}}{\chi_P} & 0 \\ 0 & 0 & \frac{1}{\chi_P} & 0 \\ \frac{p_{rev}}{\chi_P} & -\frac{1}{\chi_P} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ p_a \\ \chi_P B \\ T_a \end{pmatrix} + \begin{pmatrix} \frac{T_a T}{T_a - T}\overset{*}{Q} + \frac{T\beta}{m}B^2 & 0 & \frac{T p_{irr}}{\chi_P} & -\frac{T}{T_a - T}\overset{*}{Q} \\ 0 & 0 & 0 & 0 \\ \frac{T p_{irr}}{\chi_P} & 0 & \frac{T\beta}{m\chi_P^2} & 0 \\ -\frac{T}{T_a - T}\overset{*}{Q} & 0 & 0 & \frac{T}{T_a(T_a - T)}\overset{*}{Q} \end{pmatrix}\begin{pmatrix} \frac{1}{T} \\ \frac{p_{rev}}{T} \\ 0 \\ 1 \end{pmatrix}. \tag{A.5}$$

If we perform a variable transformation to the new, purely entropic, set of variables $\boldsymbol{x} = \begin{pmatrix} V & B & S & S_a \end{pmatrix}^T$ then the GENERIC form proves to be

$$\frac{d}{dt}\begin{pmatrix} V \\ B \\ S \\ S_a \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{\chi_P} & 0 & 0 \\ -\frac{1}{\chi_P} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} p_a - p_{rev} \\ \chi_P B \\ T \\ T_a \end{pmatrix}$$

$$+\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{T\beta}{m\chi_{\mathrm{P}}^2} & \frac{p_{\mathrm{irr}}}{\chi_{\mathrm{P}}} & 0 \\ 0 & \frac{p_{\mathrm{irr}}}{\chi_{\mathrm{P}}} & \frac{T_{\mathrm{a}}}{T(T_{\mathrm{a}}-T)}\overset{*}{Q}+\frac{\beta}{Tm}B^2 & -\frac{1}{T_{\mathrm{a}}-T}\overset{*}{Q} \\ 0 & 0 & -\frac{1}{T_{\mathrm{a}}-T}\overset{*}{Q} & \frac{T}{T_{\mathrm{a}}(T_{\mathrm{a}}-T)}\overset{*}{Q} \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}. \tag{A.6}$$

In this latter realization, the reversible operator $\boldsymbol{L}$ is simpler and is state-independent – see the Discussion on its benefits.

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