An extended dissipative particle dynamics model

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An extended dissipative particle dynamics model

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Abstract. – The method of dissipative particle dynamics (DPD) was introduced by Hoogerbrugge and Koelman (*Europhys. Lett.*, **19** (1992) 155) to study meso-scale material processes. The theoretical investigation of the DPD method was initiated by Espanol (*Phys. Rev. E*, **52** (1995) 1734) who used a Fokker-Planck formulation of the DPD method and applied the Mori-Zwanzig projection operator calculus to obtain the equations of hydrodynamics for DPD. A current limitation of DPD is that it requires a clear separation of scales between the resolved and unresolved processes. In this letter, we suggest a simple extension of DPD that allows for inclusion of unresolved stochastic processes with exponentially decaying variance for any value of the decay rate, and give an application of this algorithm to the simulation of the shallow-water equations using the Hamiltonian particle-mesh method. The proposed extension is as easy to implement as the standard DPD methods.

Dissipative particle dynamics. – Following the notation of Espanol [1], the standard DPD method of Hoogerbrugge and Koelman [2] can be formulated as a stochastic differential equation (SDE):

$$\mathrm{d}\boldsymbol{r}_i = \frac{\boldsymbol{p}_i}{m_i}\,\mathrm{d}t, \tag{1}$$

$$\mathrm{d}\boldsymbol{p}_i = \left[\boldsymbol{F}_i - \gamma\sum_{j\neq i}\omega\big(r_{ij}\big)\big(\boldsymbol{e}_{ij}\cdot\boldsymbol{v}_{ij}\big)\boldsymbol{e}_{ij}\right]\mathrm{d}t + \sigma\sum_{j\neq i}\omega^{1/2}\big(r_{ij}\big)\boldsymbol{e}_{ij}\,\mathrm{d}W_{ij}, \tag{2}$$

where m_i is the mass of particle i with position vector $\boldsymbol{r}_i = (x_i, y_i, z_i)^T$, $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$, $\boldsymbol{e}_{ij} = \boldsymbol{r}_{ij}/r_{ij}$, $\boldsymbol{v}_{ij} = \boldsymbol{v}_i - \boldsymbol{v}_j$, $\boldsymbol{v}_i = \boldsymbol{p}_i/m_i$, and $\boldsymbol{F}_i$ is the conservative force acting on particle i. The dimensionless weight function $\omega(r)$ can be chosen in a rather arbitrary manner. However, to reproduce the constant temperature macro-canonical ensemble, the friction coefficient γ and the noise amplitude σ have to satisfy the fluctuation dissipation relation

$$\sigma = \sqrt{2k_{\mathrm{B}}T\gamma},$$

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where T is the temperature of the equilibrium state and k_{B} is Boltzmann's constant. Finally, $W_{ij}(t) = W_{ji}(t)$ are independent Wiener processes.

Let us write eqs. (1)-(2) in a more compact and general manner:

$$\mathrm{d}\boldsymbol{r} = \boldsymbol{M}^{-1}\boldsymbol{p}\,\mathrm{d}t, \tag{3}$$

$$\mathrm{d}\boldsymbol{p} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r})\,\mathrm{d}t - \sum_{k=1}^{K} \nabla_{\boldsymbol{r}} h_k(\boldsymbol{r}) \Big[\gamma \dot{h}_k(\boldsymbol{r})\mathrm{d}t + \sigma\,\mathrm{d}W_k\Big], \tag{4}$$

where $\boldsymbol{r}$ is the collection of the N particle position vectors $\boldsymbol{r}_i$, $\boldsymbol{p}$ is the associated momentum vector, $\boldsymbol{M}$ is the diagonal mass matrix, $\boldsymbol{v} = \boldsymbol{M}^{-1}\boldsymbol{p}$, $V(\boldsymbol{r})$ is the potential energy,

$$\dot{h}_k(\boldsymbol{r}) = \nabla_{\boldsymbol{r}} h_k(\boldsymbol{r}) \cdot \boldsymbol{v},$$

and the functions $h_k(\boldsymbol{r})$ can again be chosen quite arbitrarily.

The choice

$$h_k(\boldsymbol{r}) = \phi(r_{ij}), \qquad \phi'(r) = \omega^{1/2}(r),$$

$k = 1, \ldots, (N-1)N/2$, in (4) leads back to the standard DPD model. However, one can also set $K = 3N$ and

$$h_i(\boldsymbol{r}) = x_i, \qquad h_{i+N}(\boldsymbol{r}) = y_i, \qquad h_{i+2N}(\boldsymbol{r}) = z_i,$$

$i = 1, \ldots, N$, in (4), which leads to the standard Langevin model

$$\mathrm{d}\boldsymbol{r} = \boldsymbol{M}^{-1}\boldsymbol{p}\,\mathrm{d}t, \tag{5}$$

$$\mathrm{d}\boldsymbol{p} = -\big[\nabla_{\boldsymbol{r}} V(\boldsymbol{r}) + \gamma \boldsymbol{v}\big]\mathrm{d}t + \sigma\,\mathrm{d}\boldsymbol{W}, \tag{6}$$

where $\boldsymbol{W}(t)$ is now a N-vector of independent random Wiener processes. Yet another variant of (4) is obtained in the context of the Hamiltonian particle mesh (HPM) method [3,4], which itself is an application of the classical particle-in-cell (PIC) or particle-mesh methods [5, 6] to geophysical fluid dynamics (GFD) [7]. Here the functions $h_k(\boldsymbol{r})$ would refer to some cell averaged quantity and k would be its cell index. For example, the fluid density at a grid point $\boldsymbol{x}_k$ can be approximated by

$$h_k(\boldsymbol{r}) = \sum_{i=1}^{N} m_i \psi\big(|\boldsymbol{x}_k - \boldsymbol{r}_i|\big),$$

with $\psi(r)$ some proper shape function such as a tensor product cubic B-spline. We will come back to this application in a later section.

We finally mention an application to molecular dynamics (MD) suggested by Ma and Izaguirre [8]. Here the stochastic part of the dynamics is used to stabilize long-time step methods and the functions h_k correspond to entries in the MD potential energy function. For example, if one would like to stabilize a bond stretching mode between atoms i and j, then $h_k(\boldsymbol{r}) = |\boldsymbol{r}_i - \boldsymbol{r}_j|$.

Generalized DPD dynamics. – Several problems, such as the Kac-Zwanzig heat bath models (see, *e.g.*, [9–11]), lead to generalized (non-Markovian) Langevin equations of type

$$\dot{\boldsymbol{r}} = \boldsymbol{M}^{-1}\boldsymbol{p}, \tag{7}$$

$$\dot{\boldsymbol{p}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}) - \int_0^t \mathcal{K}(t-s)\boldsymbol{v}\,\mathrm{d}s + \boldsymbol{U}(t), \tag{8}$$

where $\mathcal{K}(\tau)$ is a memory kernel and $\boldsymbol{U}(t)$ is an N-vector of independent and stationary zero-mean Gaussian processes. It is natural and possible to apply the same generalization to the

standard DPD model. It is important, however, that such a generalized model should still satisfy local conservation of momentum (Newton's third law). This idea leads us to consider the equations:

$$\dot{\boldsymbol{r}} = \boldsymbol{M}^{-1}\boldsymbol{p}, \tag{9}$$

$$\dot{\boldsymbol{p}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}) - \sum_{k=1}^{K} \nabla_{\boldsymbol{r}} h_k(\boldsymbol{r}) \left[\int_0^t \mathcal{K}_k(t-s)\dot{h}_k\big(\boldsymbol{r}(s)\big)\,\mathrm{d}s + U_k(t) \right], \tag{10}$$

where $\mathcal{K}_k(\tau)$, $k = 1, \ldots, K$, are again memory kernels and $U_k(t)$ are stationary zero-mean Gaussian processes. The auto-covariance functions satisfy the fluctuation dissipation relation

$$\mathbb{E}\big[U_k(t)U_k(s)\big] = k_{\mathrm{B}}T\mathcal{K}_k(t-s).$$

The following argument helps to further illuminate the generalized DPD equations (9)-(10). Define $\boldsymbol{h}(\boldsymbol{r}) = (h_1(\boldsymbol{r}), \ldots, h_K(\boldsymbol{r}))^T$ as a new variable and introduce its conjugate momenta, denoted by $\boldsymbol{p}_h$. Set $V = 0$ for a moment. Then (9)-(10) leads to generalized Langevin equations of type (7)-(8) in $(\boldsymbol{h}, \boldsymbol{p}_h)$ with the matrix $\boldsymbol{M}^{-1}$ replaced by $[\nabla_{\boldsymbol{r}}\boldsymbol{h} \cdot \boldsymbol{M}^{-1}\nabla_{\boldsymbol{r}}\boldsymbol{h}]$, which we assume to be constant for simplicity of argument.

It is convenient to approximate non-Markovian generalised Langevin dynamics models by higher-dimensional SDEs as discussed in detail by Mori [12, 13] (see also Kupferman [9]). In this note we only consider the special case of exponentially decaying kernels

$$\mathcal{K}_k(\tau) = \lambda_k e^{-\alpha_k|\tau|},$$

where α_k is the decay rate and λ_k is a scaling (coupling) parameter. In this case, then $U_k(t)$ are Ornstein-Uhlenbeck (OU) processes and the integro-differential equations (9)-(10) can be reformulated as the following SDE:

$$\mathrm{d}\boldsymbol{r} = \boldsymbol{M}^{-1}\boldsymbol{p}\,\mathrm{d}t, \tag{11}$$

$$\mathrm{d}\boldsymbol{p} = -\left[\nabla_{\boldsymbol{r}} V(\boldsymbol{r}) + \sum_{k=1}^{K} \nabla_{\boldsymbol{r}} h_k(\boldsymbol{r}) s_k\right]\mathrm{d}t, \tag{12}$$

$$\mathrm{d}s_k = -\big[\alpha_k s_k - \lambda_k \dot{h}_k(\boldsymbol{r})\big]\mathrm{d}t + \sqrt{2k_{\mathrm{B}}T\lambda_k\alpha_k}\,\mathrm{d}W_k, \quad k = 1, \ldots, K, \tag{13}$$

where $W_k(t)$ is a Wiener process for each k.

We call eqs. (11)-(13) the extended dissipative particle dynamics (EDPD) model. The standard DPD model (3)-(4) can be recovered in the limit of $\alpha \gg 1$ subject to $\lambda/\alpha = \text{const}$, in which case eq. (13) reduces to

$$s_k\,\mathrm{d}t = \frac{\lambda}{\alpha}\dot{h}_k(\boldsymbol{r})\mathrm{d}t + \sqrt{\frac{2k_{\mathrm{B}}T\lambda}{\alpha}}\,\mathrm{d}W_k$$

and we identify $\gamma = \lambda/\alpha$ and $\sigma = \sqrt{2k_{\mathrm{B}}T\lambda/\alpha}$. A rigorous proof of this statement could be performed along the lines of [14].

Generalized DPD models for other Markovian memory kernels can be found following [9, 11, 13, 15].

Time discretizations for the EDPD model. – The following modification of the popular Störmer-Verlet method [16] suggests itself:

$$\boldsymbol{p}^{n+1/2} = \boldsymbol{p}^n - \frac{\Delta t}{2}\left[\nabla_{\boldsymbol{r}} V(\boldsymbol{r}^n) + \sum_k \nabla_{\boldsymbol{r}} h_k(\boldsymbol{r}^n) s_k^n\right], \tag{14}$$

$$\boldsymbol{r}^{n+1} = \boldsymbol{r}^n + \Delta t \boldsymbol{M}^{-1}\boldsymbol{p}^{n+1/2}, \tag{15}$$

$$(1+\alpha_k\Delta t)s_k^{n+1} = s_k^n + \lambda_k\big[h_k(\boldsymbol{r}^{n+1}) - h_k(\boldsymbol{r}^n)\big] + \sqrt{2k_{\mathrm{B}}T\lambda_k\alpha_k\Delta t}\,w_k^{n+1}, \tag{16}$$

$$\boldsymbol{p}^{n+1} = \boldsymbol{p}^{n+1/2} - \frac{\Delta t}{2}\left[\nabla_{\boldsymbol{r}} V\big(\boldsymbol{r}^{n+1}\big) + \sum_k \nabla_{\boldsymbol{r}} h_k\big(\boldsymbol{r}^{n+1}\big) s_k^{n+1}\right], \tag{17}$$

where $w_k^{n+1} \sim \mathcal{N}(0,1)$ are independent random variables.

One can formally consider the DPD limit $\alpha_k \to \infty$ subject to $\lambda_k/\alpha_k = \gamma_k = \text{const}$ and $\Delta t = \text{const}$. A straightforward calculation yields the limiting scheme

$$\boldsymbol{p}^{n+1/2} = \boldsymbol{p}^n - \frac{\Delta t}{2}\left[\nabla_{\boldsymbol{r}} V(\boldsymbol{r}^n) + \sum_k \nabla_{\boldsymbol{r}} h_k(\boldsymbol{r}^n) s_k^n\right], \tag{18}$$

$$\boldsymbol{r}^{n+1} = \boldsymbol{r}^n + \Delta t \boldsymbol{M}^{-1}\boldsymbol{p}^{n+1/2}, \tag{19}$$

$$s_k^{n+1} = \frac{\gamma_k}{\Delta t}\big[h_k(\boldsymbol{r}^{n+1}) - h_k(\boldsymbol{r}^n)\big] + \sqrt{2k_{\mathrm{B}}T\gamma_k/\Delta t}\,w_k^{n+1}, \tag{20}$$

$$\boldsymbol{p}^{n+1} = \boldsymbol{p}^{n+1/2} - \frac{\Delta t}{2}\left[\nabla_{\boldsymbol{r}} V\big(\boldsymbol{r}^{n+1}\big) + \sum_k \nabla_{\boldsymbol{r}} h_k\big(\boldsymbol{r}^{n+1}\big) s_k^{n+1}\right], \tag{21}$$

which becomes identical to a scheme suggested for DPD by Groot and Warren [17] once we replace $[h_k(\boldsymbol{r}^{n+1}) - h_k(\boldsymbol{r}^n)]/\Delta t$ by $\nabla_{\boldsymbol{r}} h_k(\boldsymbol{r}^{n+1}) \cdot \boldsymbol{M}^{-1}\boldsymbol{p}^{n+1/2}$.

The scheme (14)-(17) requires only one force field evaluation per time step, conserves linear and angular momentum within the standard DPD setting, but is not symmetric (or self-consistent in the sense of Pagonabarraga, Hagen and Frenkel [18]). Hence let us replace (16) by the implicit midpoint approximation

$$\left(1+\frac{\alpha_k\Delta t}{2}\right)s_k^{n+1} = \left(1-\frac{\alpha_k\Delta k}{2}\right)s_k^n + \lambda_k\big[h_k(\boldsymbol{r}^{n+1}) - h_k(\boldsymbol{r}^n)\big] + \sqrt{2k_{\mathrm{B}}T\lambda_k\alpha_k\Delta t}\,w_k^{n+1/2},$$

where $w_k^{n+1/2} \sim \mathcal{N}(0,1)$ are again independent random variables. The new combined scheme is now clearly symmetric and not more expensive than (14)-(17).

Let us investigate the limit $\alpha_k\Delta t \gg 1$. After a few straightforward calculations one derives the limiting equations (18)-(21) with (20) replaced by

$$\frac{s_k^{n+1}-s_k^{n-1}}{2\Delta t} = -\gamma_k\frac{h_k\big(\boldsymbol{r}^{n+1}\big)-2h_k(\boldsymbol{r}^n)+h_k\big(\boldsymbol{r}^{n-1}\big)}{\Delta t^2} + \sqrt{2k_{\mathrm{B}}T\gamma_k/\Delta t}\,\frac{w_k^{n+1/2}-w_k^{n-1/2}}{\Delta t}\,. \tag{22}$$

Upon ignoring the noise term for a moment, we find that (22) corresponds to an explicit midpoint discretization in s_k of

$$\frac{\mathrm{d}}{\mathrm{d}t}s_k = -\gamma_k\frac{\mathrm{d}^2}{\mathrm{d}t^2}h_k(\boldsymbol{r}).$$

However, the explicit midpoint method is known to be unconditionally unstable. This has the implication that the symmetric variant of (14)-(17) cannot be used with a step-size $\Delta t \gg 1/\alpha_k$.

On the other hand, the symmetric scheme is superior to (14)-(17) whenever an accurate resolution of the dynamics with a step-size $\Delta t \ll 1/\alpha_k$ is desired. This situation is similar to the behavior of the BBK scheme [19] for the standard Langevin equations in the Brownian dynamics limit $\gamma\Delta t \to \infty$ and $\Delta t = \text{const}$ (see, for example, Skeel and Izaguirre [20]). Note that the self-consistent scheme of Pagonabarraga, Hagen and Frenkel [18] becomes equivalent to the BBK scheme when applied to the standard Langevin equations (5)-(6).

A numerical experiment. – In [3], Frank, Gottwald and Reich suggested a particle-mesh method, called the Hamiltonian particle-mesh (HPM) method, for the solution of the two-dimensional rotating shallow-water equations (SWEs). The Lagrangian formulation of the SWEs is

$$\ddot{\boldsymbol{X}} = -f_0\dot{\boldsymbol{X}}^{\perp} - c_0^2\nabla_{\boldsymbol{X}}h(\boldsymbol{X}),$$

where $\boldsymbol{X} = (X, Y)^T$ are the particle positions, $\dot{\boldsymbol{X}}^{\perp} = (\dot{Y}, -\dot{X})^T$. The layer depth h is given by the convolution

$$h(\boldsymbol{x}, t) = \int h_0(\boldsymbol{a})\delta(\boldsymbol{x} - \boldsymbol{X}(\boldsymbol{a}, t))\mathrm{d}\boldsymbol{a},$$

where $\boldsymbol{a} = \boldsymbol{X}(\boldsymbol{a}, 0)$ are the initial particle positions and $h_0(\boldsymbol{a})$ is the initial layer depth at $\boldsymbol{a}$. See [3, 4] for more details and [7] for the significance of the shallow-water model to GFD.

The HPM method may be viewed as an accurate numerical discretisation of the regularised fluid equations:

$$\ddot{\boldsymbol{X}} = -f_0\boldsymbol{X}^{\perp} - c_0^2\nabla_{\boldsymbol{X}}\mathscr{A} * h(\boldsymbol{X}),$$

where $\mathscr{A}$ is a smoothing operator. For later reference we denote the numerically unresolved part of the layer depth by

$$\eta = h - \mathscr{A} * h. \tag{23}$$

We next give a brief summary of the HPM method. One introduces a regular grid $\boldsymbol{x}_{kl} = (k\Delta x, l\Delta y)^T$, particles $\boldsymbol{X}_i = (X_i, Y_i)^T$, grid-centred basis functions $\psi_{kl}(\boldsymbol{X})$, and the layer depth approximation

$$\tilde{h}_{kl}(t) = \sum_{i=1}^{N} m_i\psi_{kl}(\boldsymbol{X}_i)$$

at $\boldsymbol{x}_{kl}$. The basis functions form a partition of unity, *i.e.* $\sum_{k,l}\psi_{kl}(\boldsymbol{x}) = 1$. The smoothing operator $\mathscr{A}$ is now defined as the discretization of the inverse modified Helmholtz operator with smoothing length $\Lambda = 4\Delta x$ over the grid $\boldsymbol{x}_{kl}$. The discrete approximation is denoted by $\{a_{kl}^{mn}\}$. Consequently, the finite-dimensional Hamiltonian equations of motion are given by

$$\ddot{\boldsymbol{X}}_i = -f_0\dot{\boldsymbol{X}}_i^{\perp} - c_0^2\sum_{k,l}\nabla_{\boldsymbol{X}_i}\psi_{kl}(\boldsymbol{X}_i)h_{kl}, \qquad h_{kl} = \sum_{m,n}a_{kl}^{mn}\tilde{h}_{mn}.$$

For further implementation details see again [3, 4].

We now model the numerically unresolved gravity waves in the layer depth, given by (23), with a generalized Langevin process. This idea can be mathematically motivated by representing η as the solution of a linear wave equation coupled to the particle system and subsequent reduction following the Kac-Zwanzig approach (see [11] and references therein, as well as [21]). The assumption of exponentially decaying kernel (which can be obtained by assuming that

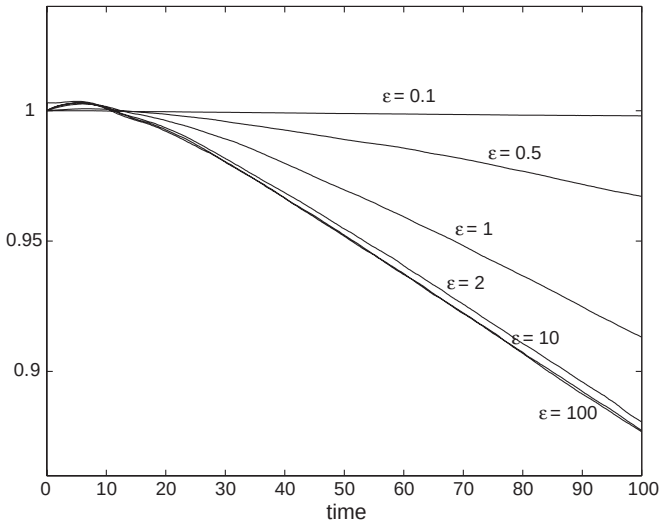

Fig. 1 – Decay of scaled energy $E(t)/E(0)$ for various values of the parameter ϵ. The value $\epsilon = 1$ is the most realistic one in the context of the shallow-water equations. The limit $\epsilon \gg 1$ corresponds to the standard DPD model.

the waves are "localised") leads to the EDPD extension of the HPM equations given below:

$$\mathrm{d}\boldsymbol{X}_i = \boldsymbol{V}_i \,\mathrm{d}t, \tag{24}$$

$$\mathrm{d}\boldsymbol{V}_i = -f_0 \boldsymbol{V}_i^{\perp} \,\mathrm{d}t - c_0^2 \sum_{k,l} [h_{kl} + s_{kl}] \nabla_{\boldsymbol{X}_i} \psi_{kl}(\boldsymbol{X}_i) \,\mathrm{d}t, \tag{25}$$

$$\mathrm{d}s_{kl} = [-\alpha s_{kl} + \lambda p_{kl}]\mathrm{d}t + c_0^{-1} (2 k_{\mathrm{B}} T \alpha \lambda)^{1/2} \,\mathrm{d}W_{kl}, \tag{26}$$

where p_{kl} is defined by

$$p_{kl} = \sum_i m_i \nabla_{\boldsymbol{X}_i} \psi_{kl}(\boldsymbol{X}_i) \cdot \boldsymbol{V}_i.$$

The only necessary modification is a scaling of the term multiplying $\mathrm{d}W_{kl}$ by c_0^{-1}. The scaling is necessary because c_0^2 multiplies the force term in (25). It should be noted that this extended model still preserves circulation (see Frank and Reich [4]).

The parameter values $f_0 = 2\pi$, $c_0 = 2\pi$, a mesh-size $\Delta x = \Delta y = 2\pi/64$, and a total of $N = 65536$ particles are used in the numerical experiments. The initial conditions for $\boldsymbol{X}_i$ and $\boldsymbol{V}_i$ correspond to an unstable shear flow and are chosen as in [3]. We set $k_{\mathrm{B}}T = 4 \times 10^{-4}$, $\lambda = \epsilon \Lambda^2$ and $\alpha = \epsilon \Lambda / c_0$ with ϵ as a free parameter and $\Lambda = 4\Delta x$. This choice corresponds to $\gamma = \Lambda^3 / c_0$ in the standard DPD method. We also have $r_{kl}(0) \sim \mathcal{N}(0, (k_{\mathrm{B}}T\lambda)^{1/2}/c_0)$. Experiments are conducted for values of ϵ varying between $\epsilon = 0.1, \ldots, 10$. The value $\epsilon = 1$ is the most natural choice [21]. Varying ϵ allows us to demonstrate the importance of the finite decay of correlation in the EDPD model with the standard DPD model corresponding to $\epsilon \gg 1$.

One should keep in mind that the initial data for the macroscopic variables are far from thermal equilibrium. In fact, for the given initial conditions and parameters, the particles lose

energy to the heat bath. This can be seen from the decay of the total particle energy,

$$E = \frac{1}{2}\sum_i m_i \left\|\dot{\boldsymbol{X}}\right\|^2 + \frac{c_0^2}{2}\sum_{k,l}\tilde{h}_{kl}(h_{kl}-1),$$

which is a conserved quantity for the HPM method. In fig. 1, we plot the decay of the scaled energy $E(t)/E(0)$ for various values of ϵ. We note that the decay rate changes dramatically for $\epsilon \in [0.1, 2]$, while for $\epsilon \geq 10$ the energy decay rate becomes independent of ϵ. This is the regime where the standard DPD method gives essentially identical results.

Conclusion. – The proposed EDPD method allows one to take into account a finite temporal decay of correlation in the unresolved degrees of freedom. A couple of numerical schemes have been suggested that are as easy to implement (and in case of self-consistency even easier) as the standard DPD algorithms available in the literature. It has been demonstrated theoretically and numerically that the limit $\alpha \to \infty$ subject to constant $\gamma = \lambda/\alpha$ leads back to the standard DPD model. The effect of finite decay of correlation on the energy decay has been demonstrated for the two-dimensional rotating shallow-water equations.

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