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SMOOTHED-PARTICLE HYDRODYNAMICS AND NONEQUILIBRIUM MOLECULAR DYNAMICS

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Abstract:

Gingold, Lucy, and Monaghan invented a grid-free version of continuum mechanics, "smoothed-particle hydrodynamics", in 1977. It is a likely contributor to "hybrid" simulations combining atomistic and continuum simulations. We describe applications of this particle-based continuum technique from the closely-related standpoint of nonequilibrium molecular dynamics. We compare chaotic Lyapunov spectra for atomistic solids and fluids with those which characterize a two-dimensional smoothed-particle fluid system.

1. Motivation

Ever since its invention, *smoothed-particle hydrodynamics* has mainly been applied to astrophysical problems (Monaghan, 1992; Lucy, 1977). More recently, it has been applied to penetration and instability problems arising in weapons design (Trease, 1991). This innovative method has also a largely-untapped potential for a variety of hybrid atomistic+continuum problems in materials science.

The "smoothed-particle method" can be imagined either to interpolate, or, alternatively, to average, solutions of the continuum partial differential equations within or upon an irregular grid. The grid point locations coincide with the centers of mass of moving lumps of material called smoothed particles. Replacing the continuous field variables {density, velocity, energy, pressure, heat flux, ...} with the resulting interpolated-or-averaged point functions at a discrete set of "particles" results in *ordinary* differential equations of motion for these particles. These equations of motion bear a strong resemblance to those of ordinary *molecular dynamics*, and so the smoothed-particle method appears to be a useful partner in hybrid simulation schemes in which atomistic and continuum particles interact. Effective hybrid schemes (Hoover, 1992) are particularly welcome in solving problems where brittle

or ductile fracture needs to be treated on an atomistic level, while the complete sample undergoing fracture is itself far too large for an exhaustive microscopic representation (Kallman, 1993).

We sketch the implementation of the method to continuum problems, but with this analogy to molecular dynamics in mind, pointing out parallel details and describing some results. Our goal here is to help render this continuum method accessible and understandable to those whose interest lies in the engineering property of materials, with an assumed background in classical many-body mechanics, "molecular dynamics".

2. Continuum Equations

Isolated systems *conserve* mass, momentum, and energy. The corresponding conservation principles are equally fundamental to the atomistic and continuum points of view. A continuum solution of the corresponding conservation equations requires (i) a material description, (ii) initial conditions, and (iii) boundary conditions. In the atomistic case the material description is a recipe for the accelerations in terms of the coordinates. These accelerations are the mechanism for the transfer of momentum and energy between particles in an atomistic system. In the continuum case the "constitutive relations" formulate the comoving fluxes of momentum and energy, the pressure tensor and the heat flux vector, in terms of velocity and energy (temperature) gradients.

The continuum equations describing the flow of mass, momentum, and energy must account for additional flux contributions due to the relative motion of the described material and the describing coordinate system. The form of the equations to be solved is naturally simplest in the Lagrangian comoving frame where the convective contributions to the fluxes vanish. This is also the natural frame for describing smoothed particles which, like atoms, follow the motion. Conservation of mass, momentum, and energy lead directly to the fundamental equations of continuum mechanics: the "continuity equation", the "equation of motion", and the "energy equation":

$$d\rho/dt \equiv \partial\rho/\partial t + v\cdot\nabla\rho = -\rho\nabla\cdot v \; ;$$

$$\rho dv/dt \equiv \rho\partial v/\partial t + \rho v\cdot\nabla v = -\nabla\cdot P \; ;$$

$$\rho de/dt \equiv \rho\partial e/\partial t + \rho v\cdot\nabla e = -P:\nabla v - \nabla\cdot Q \; .$$

3. Averages and Gradients using Smoothed-Particle Hydrodynamics

The smoothed-particle form of the continuum equations gives the time development of particle trajectories, representing the flow, in terms of the gradients of the stress tensor, the energy, and their gradients, as well as the velocity gradient, and the divergence of the heat flux vector. The smoothed-particle approach transforms the *partial* differential continuum equations to *ordinary* differential equations of motion for particles. These particles have a *fixed* mass m, distributed in space according to a normalized weighting function w(r). At the same time they are characterized by a *varying* density ρ, computed by adding the contributions from nearby particles' weighting functions to each particle's own contribution, mw(0).

The smoothed-particle approach (Monaghan, 1992; Lucy, 1977) to solving the continuum equations begins with the *definition* of the smoothed average <f> of a field variable f, at a location I:

$$<f>_I \equiv \Sigma m_J w_{IJ} f_J / \rho_J \; ; \; \rho_J \equiv \Sigma m_K w_{JK} \; .$$

The equivalent definition of the averaged gradient <∇f> follows by differentiation of the definition for $<f>_I$:

$$<\nabla f>_I \equiv \Sigma m \nabla_I w_{IJ} f_J / \rho_J \; .$$

The continuum equations of motion also require the strain-rate tensor (the symmetrized velocity-gradient), $\nabla v + \nabla v^t$, which can most conveniently be evaluated from the identity:

$$\rho \nabla v \equiv [\nabla(\rho v) - v \nabla \rho] \; .$$

Applying the smoothed-particle definition of gradient, the two gradients on the righthand side of the velocity-gradient-tensor expression can be combined to give a sum over the relative velocity of each IJ pair:

$$\rho_I <\nabla v>_I \equiv m\Sigma[\nabla_I w_{IJ} v_J - v_I \nabla_J w_{IJ}] \equiv - m\Sigma \nabla_I w_{IJ} v_{IJ} \; ; \; v_{IJ} \equiv v_I - v_J \; .$$

Because the weighting function w vanishes for r = ±dr, it is clear that the *first* nonvanishing term in the Taylor's series expansion of the sums is, when approximated by an integral, proportional to the velocity gradient. The next set of nonvanishing (third-order) terms provides effective

"super-Burnett" transport coefficients. These coefficients are ordinarily too small to observe, but it is possible that an investigation of alternative difference expressions for the gradients would yield useful results for shockwave structure. In shockwaves the deviations from the predictions of linear transport theory are significant (Holian, 1980).

The contribution of an IJ pair of smoothed particles to the local temperature gradient, required to calculate the heat-flux vector Q, can be written in an analogous way, and then used to evaluated the divergence of the heat flux, which provides the conductive part of $\{de/dt\}$. In our own work we have used Monaghan's constant-conductivity, constant-heat-capacity formulation of conduction. We plan to explore the more-realistic elaborations of this simplest model in the near future.

With the velocity and temperature gradients evaluated, the smoothed-particle method can be applied to any problem described by the Navier-Stokes equations. We will illustrate such simulations with some simple examples after sketching the details of the corresponding simulation program.

4. Simulation Program with Smoothed-Particle Hydrodynamics

In molecular dynamics the system's state is described by the coordinate and velocity sets $\{r\}$ and $\{v\}$. A simulation (Hoover, 1991, 1992; Kallman, 1993; Holian, 1980; Allen, 1987) proceeds by solving the first-order equations for $\{dr/dt\}$ and $\{dv/dt\}$ or the second-order equations for $\{d^2r/dt^2\}$. The continuum situation is more complicated. First, there are the additional variables, such as the densities $\{\rho\}$ and the internal energies $\{e\}$ entering into the equations of motion. Second, the motion ordinarily incorporates contributions from the gradients $\{\nabla v, \nabla T\}$ as well. Storage requirements are increased further by the need to accumulate stress tensors and heat-flux vectors at each particle site.

Our FORTRAN computer programs implementing smoothed-particle hydrodynamics are based on the following general approach:

1. Initialize particle properties $\{r,v,e\}$; set $\{dr/dt\} = \{v\}$.
2. Compute $\{\rho\}$ from the coordinates and weight functions $\{w_{IJ}\}$.
3. Find the boundary energies $\{e\}$ to match specified boundary $\{\rho,T\}$.
4. Calculate the constitutive properties, including transport coefficients:
   $\{P_{EQUILIBRIUM}(\rho,e) \equiv -\sigma_{EQUILIBRIUM}(\rho,e), \eta(\rho,e), \eta_{BULK}(\rho,e), \kappa(\rho,e)\}$.
5. Compute $\{\nabla v, \nabla T\}$.
6. Calculate $\{\sigma, Q, \nabla\cdot\sigma, \nabla\cdot Q\}$ $\{dv/dt, de/dt\}$ including boundary conditions .
7. Use the complete set $\{dr/dt, dv/dt, de/dt\}$ to advance the time by dt .

We have found it to be convenient to assign these steps to separate subroutines, and to guard against numerical errors by using the classic Fourth-Order Runge-Kutta integrator. The weighting function w, equilibrium equations of state P(ρ,e), T(ρ,e), e(ρ,T), and the state-dependent transport coefficients $\{\eta,\eta_{BULK},\kappa\}$ are likewise relegated to subroutines. We have mostly used very smooth (continuous second derivative) weighting functions taken from Monaghan's (1992) and Lucy's (1977) work, as well as a more-localized weighting function with a cusp at the origin. For a radial coordinate range of dr, and with the normalization, $\int 2\pi w r dr \equiv 1$, appropriate to two space dimensions, these functions have the forms:

$$w_M(0<x<1/2) \equiv (40/7\pi dr^2)(1 - 6x^2 + 6x^3) ,$$

$$w_M(1/2<x<1) \equiv (80/7\pi dr^2)(1 - x)^3 ;$$

$$w_L(0<x<1) \equiv (5/\pi dr^2)(1 + 3x)(1 - x)^3 ;$$

$$w_C(0<x<1) \equiv (10/\pi dr^2)(1 - x)^3 ,$$

where $x = r/dr$ is a reduced length [with $0 < x < 1$]. The Monaghan, Lucy, and Cusp weighting functions are shown in **Figure 1.**

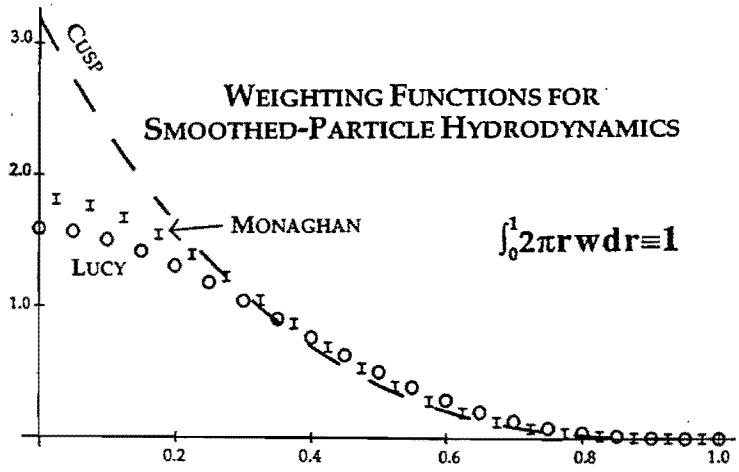


Figure 1. Weighting functions w(r) used in two-dimensional smoothed-particle hydrodynamics. Lucy's and Monaghan's functions have continuous second derivatives. The cusp function tends to reduce the number of pairs of particles at small separations.

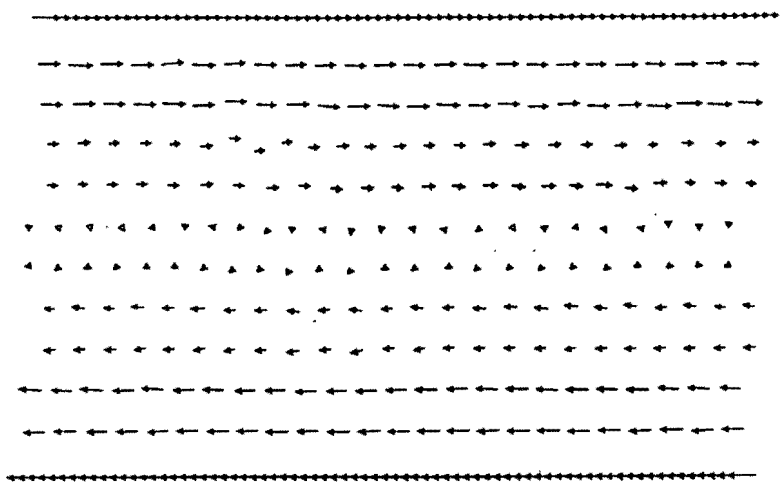


Figure 2. A smoothed-particle system with two fixed horizontal rows of boundary particles and with periodic boundaries at the sides, so that particles "leaving" the system's right/left sides are reintroduced on the opposite left/right sides.

We have imposed boundary conditions by using boundary particles with *individually-programmed* coordinates, velocities, and energies. Ashurst's "fluid walls", in which several particles, localized in space, satisfy *collective* constraints (Hoover, 1975), are a natural extension of these individually-constrained particle boundaries. As tests, we have considered two prototypical cases corresponding to the system shown in **Figure 2**. The simpler case is ordinary heat conduction, in which neither horizontal wall moves. A slightly more complicated case is shown in **Figure 2**, plane Couette flow, in which the fluid motion is driven by parallel rows of moving boundary particles. The temperatures of the walls are held fixed in either case, so that the system settles into a nonequilibrium stationary state.

Just as in ordinary molecular dynamics simulations, the search over all N(N–1)/2 pairs of particles is prohibitively expensive, for large N. To find those relatively few pairs which are close enough to interact, particles are assigned to cells, of width equal to, or just slightly exceeding, the range of the weight function w(dr). This assignment is not particularly time-consuming, and so can be carried out at every time step.

5. Massively-Parallel Simulations with SPRINT-2 and SPRINT-3

Most of our large-system continuum mechanics and molecular dynamics work has been carried out using FORTRAN programs on Tony De Groot's massively-parallel $30,000 SPRINT-2 computer (De Groot, 1987). We have carried out atomistic and continuum simulations with millions of degrees of freedom on this machine (Hoover, 1992; Kallman, 1993). This machine pays for itself (in terms of the equivalent cost of displaced CRAY time) in only two to three days! The simulation is distributed over the 64 (SPRINT-2) or 256 (SPRINT-3) transputer-based processors by dividing the system up into a network of contiguous regions, one for each processor. The regions are in turn divided up into cells with a width slightly greater than the range of particle interactions. The properties of those cells forming a one-cell-thick "skin" at the boundary of the region controlled by a particular processor are transferred to neighboring processors. The efficiency of these calculations exceeds 90% for problems with just a few hundred particles per region. SPRINT-3, with forty times the speed of SPRINT-2 (primarily due to faster processors), is currently under construction at Livermore. The cost of this successor machine will be about $500,000.

6. Models for Testing Smoothed-Particle Simulations

Our preliminary investigations were carried out for a classical ideal gas equation of state, $PV = E = NkT$, with constant shear viscosity and heat conductivity. Because our ultimate interest lies in hybrid calculations linking together relatively-dense atomistic and continuum regions, we have also sought a simple reproducible force law model suited to both the atomistic and continuum approaches. We wanted a force law less complicated than the splines used to truncate the Lennard-Jones potential.

We chose a potential (Posch, 1989) with three vanishing derivatives at the cutoff distance, $r = \sigma$:

$$\phi(r) = 100\varepsilon[(1 - (r/\sigma)^2]^4 .$$

We choose the interaction strength equal to 100ε, so that the separation corresponding to energy ε, an effective collision diameter at a temperature equal to ε/k, is 0.8269σ. We determined the mechanical and thermal equations of state in the vicinity of unit density, $N\sigma^2 = V$, and temperature by carrying out a suite of isokinetic molecular dynamics simulations and fitting the results to quadratic forms. At unit (number) density and reduced temperature ρ, kT/ε, $PV/N\varepsilon$ and $E/N\varepsilon$ are respectively 1.00, 1.00, 5.04 and

1.44. For small deviations from this standard state, the following expansions apply:

$$PV/N\varepsilon = 5 + 8\delta\rho + 2.5\delta\varepsilon + 9\delta\rho^2 + 2\delta\rho\delta\varepsilon\,;$$

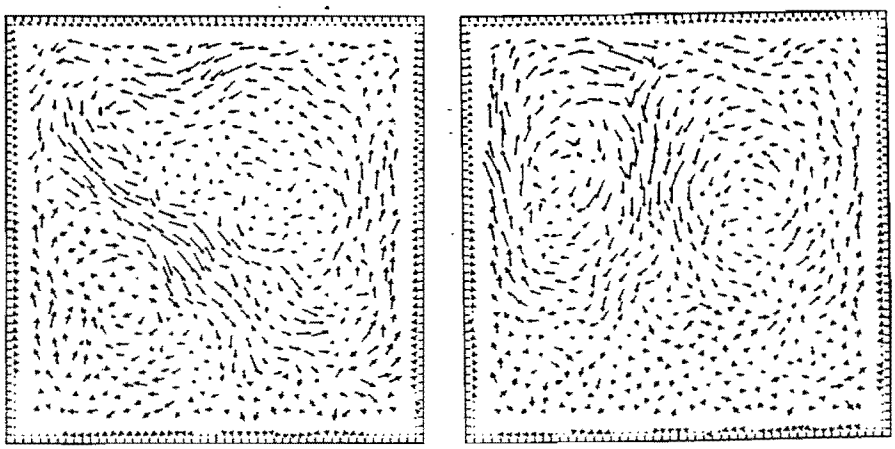
$$kT/\varepsilon = 1 - \delta\rho + 0.7\delta\varepsilon - 0.8\delta\rho^2 - 0.5\delta\rho\delta\varepsilon\,;$$

$$e/\varepsilon \equiv E/N\varepsilon = 1.443 + 1.5\delta\rho + 1.5\delta\tau + 2.4\delta\rho^2 + 1.2\delta\rho\delta\tau\,;$$

$$\delta\rho \equiv (N\sigma^2/V) - 1.000\,;\ \delta\varepsilon \equiv (E/N\varepsilon) - 1.443\,;\ \delta\tau \equiv (kT/\varepsilon) - 1.000\,.$$

The first two expansions provide local-equilibrium pressures, which contribute to the accelerations {dv/dt}, and local temperatures, which drive the heat flux. Both contribute to {de/dt}. The additional expansion of energy as a series in $\delta\rho$ and $\delta\tau$ is made necessary by our thermal boundary conditions. On the boundaries, where energy must be calculated from the observed density and a specified boundary temperature, the special thermal equation giving $E/N \equiv e(\delta\rho,\delta\tau)$ is required.

Figure 3 (below) shows two snapshots from a smoothed-particle simulation of Rayleigh-Bénard instability, using this thermodynamic equation of state with constant kinematic viscosity and thermal diffusivity. This simulation uses the "cusp" weighting function. The development of this system is characterized by a variety of recurring roll patterns, of widely differing kinetic energies.



7. Relation of Smoothed-Particle Hydrodynamics to Molecular Dynamics

There is an obvious superficial resemblance of smoothed-particle simulations to molecular-dynamics simulations. In both cases a large number of particles move, in two- or three-dimensional space, according to nonlinear ordinary differential equations of motion, with accelerations involving the interactions of near neighbors. In a particular special case, the analogy is even closer. The smoothed-particle equations of motion, written in terms of the individual-particle stress tensors $\{\sigma\}$, are (Monaghan, 1992):

$$\{ (d^2r/dt^2)_i = m(dt)^2\Sigma[(\sigma/\rho^2)_i + (\sigma/\rho^2)_j]\cdot\nabla_i w_{ij} \} .$$

In the special case that the material being described is an isentropic two-dimensional monatomic ideal gas, the stress tensor is isotropic, and proportional to ρ^2. Thus the motion of the coordinates follows from the gradient of a pairwise-additive sum of pair terms. The weighting function w(r), in this special case, plays the role of a pairwise-additive, softly-repulsive potential function, $\Phi \propto \Sigma w_{ij}$.

8. Lyapunov Spectra

The analogy linking the smoothed-particle continuum picture to atomistic molecular dynamics suggests that the smoothed-particle representation of a continuum might exhibit the same chaotic instabilities which are present in atomistic systems. These chaotic instabilities, for systems with many degrees of freedom, are best characterized through the Lyapunov spectrum (Hoover, 1991; Posch, 1989).

The biggest Lyapunov exponent describes the time-averaged rate at which two nearby phase-space trajectories separate, $\langle d\ln\delta/dt\rangle \equiv \lambda_1$. The next largest Lyapunov exponent λ_2 describes the growth in a direction orthogonal to that associated with λ_1. Thus the time-averaged growth rate of the *area* defined by three nearby trajectories defines λ_2: $\langle d\ln A/dt\rangle \equiv (\lambda_1+\lambda_2)$. The Lyapunov instability of molecular systems was first investigated by Stoddard and Ford (1973), who computed λ_1 for a two-dimensional many-body system. More recently, Posch and Hoover characterized the entire spectrum of Lyapunov exponents for equilibrium and nonequilibrium systems in both two and three space dimensions (Posch, 1989). Typical equilibrium spectra from that work are reproduced in Figure 4.

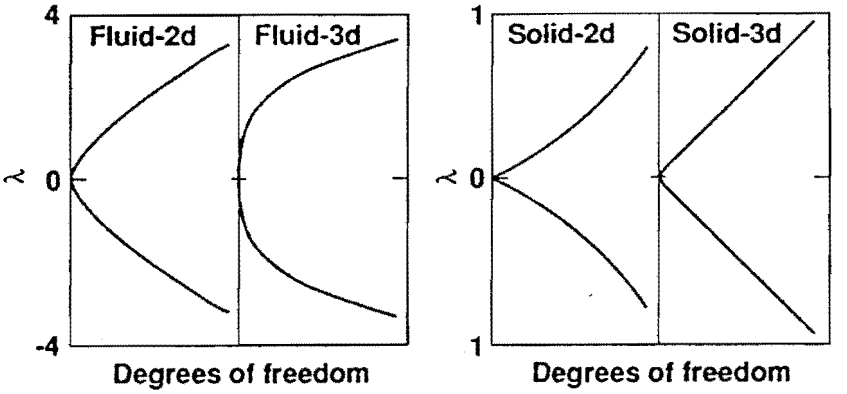


Figure 4. Typical Lyapunov spectra for two- and three-dimensional fluids and solids. A conservative system with f degrees of freedom, and with states spanning a 2f-dimensional phase space, has f pairs $\{+\lambda,-\lambda\}$ of 2f Lyapunov exponents.

The chaotic nature of discretized continuum simulations can also be described through Lyapunov spectra, though the richer variety of continuum systems and solution techniques has not yet led to any simplifying overall classification of the spectra. The smoothed-particle descriptions of continuum systems are typically chaotic, even if the underlying hydrodynamic system is relatively simple. We have investigated the simplest possible continuum case, a two-dimensional ideal gas, using smoothed-particle hydrodynamics. The energy of such a system can be described implicitly as internal energy, or, more explicitly, as the particulate kinetic energy associated with phonons.

Figure 5 shows typical Lyapunov spectra for 16-particle periodic descriptions of an ideal gas, in two space dimensions, using Lucy's weighting function, as described in **Figure 1**. The system is a rectangle, with width 4 and height $(12)^{1/2}$. Because each smoothed particle has two (x and y) space coordinates, two velocity components, and an internal energy, the state space is 80-dimensional, and is described by 40 pairs of Lyapunov exponents. Two cases are displayed. In the first, the initial internal energy of the gas is 16 and the kinetic energy is 1. In the second, this is reversed, with initial internal energy equal to 1 and kinetic energy 16. It is interesting that these dynamical spectra for a smoothed-particle description of an ideal *fluid* resembles the corresponding dynamical description, shown in Figure 4, of a two-dimensional *solid*.

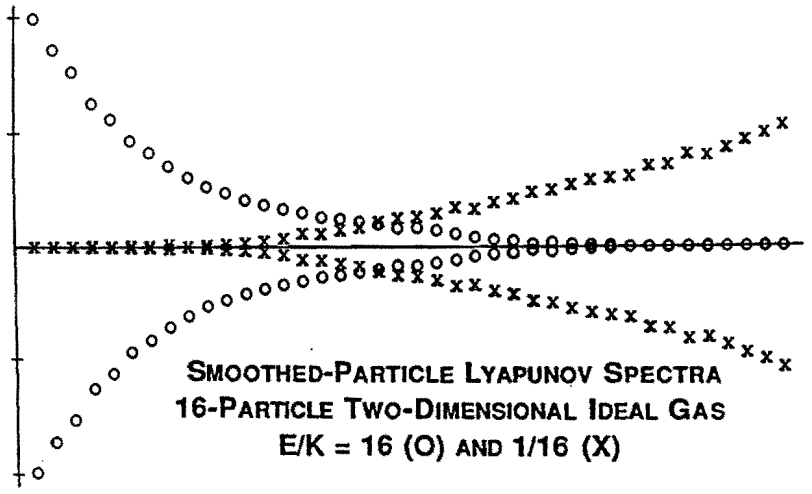


Figure 5. Smoothed-particle Lyapunov spectra, using the Lucy weighting function, for a two-dimensional periodic 16-particle ideal gas. The initial kinetic and internal energies differ by a factor of 16 in the cases shown here. For an internal-to-kinetic energy ratio of 16 (1/16) each exponent is indicated as an O (X).

9. Conclusion

The logical and computational structure of smoothed-particle hydrodynamics closely resembles that of ordinary molecular dynamics, though additional state variables are required. The dynamics, the treatment of boundary conditions, and the analysis of chaotic instability are similar too. This promising approach should prove particularly valuable in constructing hybrid methods bridging the gap between the atomistic and continuum views and in characterizing the fluctuations which underlie continuum flows.

10. Acknowledgment

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