Numerical Analysis of Deconvolution Closure for Mesoscopic Continuum Models of Particle Systems

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Presentation Overview

Problem Introduction and Motivation

We are interested in solving for the location of particles in time in a d-dimensional particle system over some short period of time T. We have $N \gg 1$ identical particles P_i on some computational domain $\Omega \in \mathbb{R}^d$. The total mass of the system is denoted M. Each particle i has some velocity $\mathbf{v}_i$ and position $\mathbf{q}_i$ and is influenced by both inter-particle and external forces.

Discrete Problem

To satisfy physical law the system of particles must satisfy a system of ordinary differential equations [1]

$$\dot{\mathbf{q}}_i = \frac{d\mathbf{q}_i}{dt} = v_i, \tag{1}$$

$$\frac{M}{N}\dot{\mathbf{v}}_i = \mathbf{f}_i + \mathbf{f}_i^{(ext)}, \tag{2}$$

subject to initial conditions,

$$\mathbf{q}_i(0) = \mathbf{x}_i, \tag{3}$$

$$\mathbf{v}_i(0) = \mathbf{v}_i^0. \tag{4}$$

Discrete Problem, cont.

Where

(i) $\mathbf{f}_i^{(ext)}$ denotes external forces (gravity, confining forces)

(ii) and $\mathbf{f}_i$ are pair interparticle forces

$$\mathbf{f}_i = \sum_j \mathbf{f}_{ij}.$$

Discrete Problem, cont.

We study asymptotic behavior as $N \to \infty$. Scaling is required to bound the amount of energy in the system independent of N. An example of this scaling is:

$$\mathbf{f}_{ij} = -\frac{1}{N}\nabla_{\mathbf{q}_i} U\left(\frac{|\mathbf{q}_i - \mathbf{q}_j|}{\varepsilon}\right) = -\frac{1}{\varepsilon N}\frac{d}{d\xi}U(\xi),$$

where forces are generated by a finite range pair potential $U(\xi)$ where ξ is the distance away from a particle.

Mesoscale Approximations

Instead of solving these ordinary differential equations directly on the microscale, we will use integral approximations for the required properties on the mesoscale. We replace the exact microscopic quantities with regularized deconvolution approximations.

Mesoscale, cont.

To find the averages, we define a windowing function, ψ, that satisfies

$$\int \psi(\mathbf{x}) d\mathbf{x} = 1.$$

To convert to the mesoscale we scale with η,

$$\psi_\eta(\mathbf{x}) = \eta^{-d} \psi \left(\frac{\mathbf{x}}{\eta} \right).$$

This window function will allow us to generate averages of micro-scale dynamical functions.

Mesoscale, cont.

By applying the windowing function we obtain our averages. The mesoscopic *average density* is:

$$\bar{\rho}^{\eta}(t,\mathbf{x}) = \frac{M}{N}\sum_{i=1}^{N}\psi_{\eta}(\mathbf{x}-\mathbf{q}_i(t)). \tag{5}$$

And the mesoscopic *average momentum* is:

$$\bar{\rho}^{\eta}\bar{v}^{\eta}(t,\mathbf{x}) = \frac{M}{N}\sum_{i=1}^{N}\mathbf{v}_i(t)\psi_{\eta}(\mathbf{x}-\mathbf{q}_i(t)). \tag{6}$$

Mesoscale, cont.

Differentiating (5) and (6) with respect to t and using (1) and (2) yields *exact mesoscopic balance equations* for the primary variables:

$$\begin{aligned}\frac{\partial}{\partial t}\bar{\rho}^{\eta}(t,\mathbf{x}) &= \frac{\partial}{\partial t}\frac{M}{N}\sum \psi_{\eta}(\mathbf{x}-\mathbf{q}_i(t)) \\ &= -\frac{M}{N}\sum \frac{\partial \psi_{\eta}}{\partial t}(\mathbf{x}-\mathbf{q}_i(t))\ \mathbf{q}_i'(t) \\ &= -\frac{M}{N}\sum \frac{\partial \psi_{\eta}}{\partial t}(\mathbf{x}-\mathbf{q}_i(t))\ \mathbf{v}_i(t)\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial t}\bar{\rho}^{\eta}\bar{\mathbf{v}}^{\eta}(t,\mathbf{x}) &= \frac{\partial}{\partial t}\frac{M}{N}\sum \mathbf{v}_i(t)\psi_{\eta}(\mathbf{x}-\mathbf{q}_i(t)) \\ &= \frac{M}{N}\left(\mathbf{v}_i'(t)\psi_{\eta}(\mathbf{x}-\mathbf{q}_i(t)) + \mathbf{v}_i(t)\frac{\partial \psi_{\eta}}{\partial t}(\mathbf{x}-\mathbf{q}_i(t))\mathbf{q}_i'(t)\right) \\ &= \frac{M}{N}\left(\mathbf{v}_i'(t)\psi_{\eta}(\mathbf{x}-\mathbf{q}_i(t)) + \mathbf{v}_i^2(t)\frac{\partial \psi_{\eta}}{\partial t}(\mathbf{x}-\mathbf{q}_i(t))\right)\end{aligned}$$

Mesoscale, cont.

Conservation of mass and momentum balance equations take the form:

$$\partial_t \bar{\rho}^\eta + \mathrm{div}(\bar{\rho}^\eta \bar{\mathbf{v}}^\eta) = 0 \quad (7)$$

$$\partial_t (\bar{\rho}^\eta \bar{\mathbf{v}}^\eta) + \mathrm{div}(\bar{\rho}^\eta \bar{\mathbf{v}}^\eta \otimes \bar{\mathbf{v}}^\eta) - \mathrm{div}\mathbf{T}^\eta = 0 \quad (8)$$

The *convective stress* is

$$\mathbf{T}^\eta_{(c)}(t, \mathbf{x}) = -\sum m_i(\mathbf{v}_i - \bar{\mathbf{v}}^\eta(t, \mathbf{x})) \otimes (\mathbf{v}_i - \bar{\mathbf{v}}_i{}^\eta(\mathbf{x}, t))\psi(\mathbf{x} - \mathbf{q}_i)$$

and the *interaction stress* is over all pairs (i, j) of particles that interact with one another.

$$\mathbf{T}^\eta(t, \mathbf{x})_{(int)} = \sum_{(i,j)} \mathbf{f}_{ij} \otimes (\mathbf{q}_j - \mathbf{q}_i) \int_0^1 \psi_\eta(s(\mathbf{x} - \mathbf{q}_j) + (1 - s)(\mathbf{x} - \mathbf{q}_i))ds$$

The total stress is then $\mathbf{T}^\eta = \mathbf{T}^\eta_{(c)} + \mathbf{T}^\eta_{int}$.

Overview of Numerical Solution

The mesoscale partial differential equations

$$\partial_t \bar{\rho}^\eta + \mathrm{div}(\bar{\rho}^\eta \bar{\mathbf{v}}^\eta) = 0,$$
$$\partial_t (\bar{\rho}^\eta \bar{\mathbf{v}}^\eta) + \mathrm{div}(\bar{\rho}^\eta \bar{\mathbf{v}}^\eta \otimes \bar{\mathbf{v}}^\eta) - \mathrm{div}\mathbf{T}^\eta = 0,$$

provide a way of approximating

$$\dot{\mathbf{q}}_i = \frac{d\mathbf{q}_i}{dt} = v_i,$$
$$\frac{M}{N}\dot{\mathbf{v}}_i = \mathbf{f}_i + \mathbf{f}_i^{(ext)},$$

applied with some potential function.

However an attempt at solving the nonlinear problem directly numerically was unstable.

Overview of Numerical Solution, cont.

To make progress, we first sought to understand the nonlinear system better.

- To this end, Dr. Panchenko linearized the mesoscale problem.
- Efforts were made to understand related linear systems and to investigate different Runge-Kutta schemes for solving these systems.
- We then implemented several numerical schemes to test the methods. It was found that the numerical methods used were not responsible for the instability.

Overview of Numerical Solution, cont.

Then we went back to the nonlinear problem.

- We produced a predictor with the linearization. The hope was that the solution would progress quickly and stably in time.
- Then we used the nonlinear problem to create a corrector. This involved solving convective and interaction stress integrals numerically.
- The predictor-corrector was implemented and tested against an associated microscale problem that was run on a cluster.

Interpolating functions

Introduce suitable interpolating functions $\tilde{v}$ for velocity and $\tilde{q}$ for position for a uniform grid $\{x_j\}$ that satisfy

$$\begin{aligned} \tilde{q}(0, x_j) &= q_j^0 \\ \tilde{v}(0, \tilde{q}(0, x_j)) &= v_j^0 \end{aligned}$$

initially and

$$\begin{aligned} \tilde{q}(t, x_j) &= q_j(t) \\ \tilde{v}(t, \tilde{q}(t, x_j)) &= v_j(t) \end{aligned}$$

at other times.

Now Interpolated

In a one-dimensional case the exact mesoscopic balance equations become

$$T^{\eta}_{(c)}(t,x) = -\frac{M}{L}\int_0^L (\tilde{v}(t,y) - \overline{v}^{\eta}(t,x))^2 \psi_\eta(x-y) J(t,y)\ dy \tag{9}$$

which is *convective stress*, and the *interaction stress* is

$$T^{\eta}_{(int)}(t,x) = -\frac{N-1}{N}\int_0^L U'\left(\frac{L}{J(t,y)}\right)\int_0^1 \psi_\eta\left(x - y - \frac{sh}{J(t,y)}\right)\ ds\ dy. \tag{10}$$

The *conservation of mass* and *momentum* equations are then

$$\partial_t \bar{\rho}^{\eta} + \partial_x(\bar{\rho}^{\eta}\overline{v}^{\eta}) = 0 \tag{11}$$

$$\partial_t(\bar{\rho}^{\eta}\overline{v}^{\eta}) + \partial_x(\bar{\rho}^{\eta}(\overline{v}^{\eta})^2) - \partial_x(\bar{T}^{\eta}_{(c)} + \bar{T}^{\eta}_{(int)}) = 0. \tag{12}$$

Linearization

In [2], Dr. Panchenko linearized (11) and (12) to obtain

$$\partial_t \tilde{\rho} + \rho_0 \partial_x \tilde{v} = 0, \quad (13)$$

$$\rho_0 \partial_t \tilde{v} - \partial_x \tilde{T}_{(int)} = 0, \quad (14)$$

where

$$\tilde{T}_{int} = -\frac{L^2}{M} \tilde{\rho} \cdot A$$

and

$$A = \sum_{p=1}^{p_*} p^2 U''(Lp).$$

Here $M > 0$ denotes the mass, $L > 0$ is the width of the interval occupied by the particles. p_* denotes the total number of particles effected and U is some potential function. Typically p_* is 2 or 3.

Linearization, cont.

The stress terms may be expressed in terms of density to become

$$\rho_0 \partial_t \tilde{v} + \frac{L^2 A}{M} \partial_x \tilde{\rho} = 0.$$

Eliminating $\tilde{\rho}$ gives the *wave equation* in terms of $\tilde{v}$

$$\partial_{tt} \tilde{v} - \frac{L^2 A}{M} \partial_{xx} \tilde{v} = 0. \tag{15}$$

Linearization, cont.

Let $c^2 = L^2 A/M$, and we have a standard wave equation that describes velocity of the velocity interpolation $\tilde{v}$ on a closed interval $x \in [0, L]$

$$\partial_{tt}\tilde{v} - c^2\partial_{xx}\tilde{v} = 0, \tag{16}$$

with initial conditions and periodic boundary conditions

$$\begin{aligned} \tilde{v}(x,0) &= f(x) = 1 \\ \tilde{v}_t(x,0) &= g(x) = v_0. \end{aligned}$$

Linearization, cont.

A solution via separation of variables will give us an analytic result to compare our numerical method against. The general solution to the wave equation is

$$\tilde{v}(x,t) = \sum_{n=1}^{N} [A_n \cos(\lambda_n t) + B_n \sin(\lambda_n t)] \sin(\frac{n\pi}{\ell} x)]$$
$$+ \sum_{n=1}^{N} [C_n \cos(\lambda_n t) + D_n \sin(\lambda_n t)] \cos(\frac{n\pi}{\ell} x)].$$

The constants A_n, B_n, C_n and D_n depend upon f, g, the initial conditions and boundary conditions. This approximated analytic solution was plotted against a Runge-Kutta numerical solution to test the viability of using Runge-Kutta to solve the wave equation.

Predictor

We will discretize the right hand side of (16) (wave equation) to put it into a matrix form Au for a Runge-Kutta method. Let $x_1 = 0$ and $x_N = L$. Define $h = x_i - x_{i-1}$, as a uniform spacing of the partition and a uniform time step as $k = t_i - t_{i-1}$. Let $\mathbf{u} = (u(x_1,t), u(x_2,t), ..., u(x_N,t))^T$ where each x_i is an element of a uniformly spaced partition $x_0 < x_1 < \ldots < x_N$. Then we obtain a $O(h^2)$ discretized system of first order equations.

$$u_{xx}(x,t) \approx \frac{u^k_{h+1} - 2u^k_h + u^k_{h-1}}{h^2}$$

Predictor, cont.

From this we obtain a matrix A that operates on $\mathbf{u}$ that discretizes the wave equation into the form $\mathbf{u}_{tt} = A\mathbf{u}$.
For the left side, we make the following substitution

$$\mathbf{v} = \mathbf{u}_t$$
$$\mathbf{v}_t = \mathbf{u}_{tt},$$

and let

$$\mathbf{U} = \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}.$$

Predictor, cont.

Then the discretization may be written as a matrix equation

$$\mathbf{U}_t = \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}_t = \begin{bmatrix} \mathbf{v} \\ A\mathbf{u} \end{bmatrix} = \begin{bmatrix} 0 & I \\ A & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} \tag{17}$$

which is suitable for a Runge-Kutta scheme.

Predictor, cont.

Strong Stability Preserving Runge-Kutta

SSP Runge-Kutta methods are suitable for solving systems of ordinary differential equations in the form

$$U_t = -f(U)_x,$$

which arise commonly in problems involving hyperbolic conservation laws. The spatial derivative is discretized to obtain $L(U)$ using finite differences or finite elements. $L(U)$ has the property that for some sufficiently small time step $\triangle t \leq \triangle t_{FE}$, which must satisfy the Courant-Friedrichs-Levy (CFL) condition, and first-order Euler time discretization

$$U^{n+1} = U^n + \triangle t L(U^n).$$

Predictor, cont.

Strong Stability Preserving Runge-Kutta, cont.

The total variation of the one-dimensional discrete solution does not increase in time. This ensures that the method maintains a strong stability property

$$TV(U^{n+1}) \leq TV(U^n) \text{ for } TV(U^n) := \sum_j |U^n_{j+1} - U^n_j|,$$

while achieving high order accuracy in time [7].

Predictor, cont.

Strong Stability Preserving Runge-Kutta, cont.

Call the block matrix $\mathbf{A}$. We will use SSPRK(3,3) as defined in [4]. This is an optimal third-order method:

$$\mathbf{U}^{(1)} = \mathbf{U}^n + \triangle t\mathbf{A}(\mathbf{U}^n)$$
$$\mathbf{U}^{(2)} = \frac{3}{4}\mathbf{U}^n + \frac{1}{4}\mathbf{U}^{(1)} + \frac{1}{4} \triangle\, t\; \mathbf{A}(\mathbf{U}^{(1)})$$
$$\mathbf{U}^{n+1} = \frac{1}{3}\mathbf{U}^n + \frac{2}{3}\mathbf{U}^{(2)} + \frac{2}{3} \triangle\, t\; \mathbf{A}(\mathbf{U}^{(2)}).$$

Predictor, cont.

Forth-Order Runge-Kutta

For comparison we also used a standard fourth-order Runge-Kutta:

$$
\begin{aligned}
\mathbf{U}^{(1)} &= \mathbf{A}\mathbf{U}^n \\
\mathbf{U}^{(2)} &= \mathbf{A}\left(\mathbf{U}^n + \frac{\triangle t}{2}\mathbf{U}^{(1)}\right) \\
\mathbf{U}^{(3)} &= \mathbf{A}\left(\mathbf{U}^n + \frac{\triangle t}{2}\mathbf{U}^{(2)}\right) \\
\mathbf{U}^{(4)} &= \mathbf{A}\left(\mathbf{U}^n + \triangle t\mathbf{U}^{(3)}\right) \\
\mathbf{U}^{n+1} &= \mathbf{U}^n + \frac{\triangle t}{6}\left(\mathbf{U}^{(1)} + 2\mathbf{U}^{(2)} + 2\mathbf{U}^{(3)} + \mathbf{U}^{(4)}\right).
\end{aligned}
$$

We can think of the initial state of the system as an $n \times 1$ vector containing all ones for each x_i, which is $\mathbf{U}^0$.

Predictor, cont.

SSPRK(3,3) vs. RK4

The vector values of $\mathbf{U}_t$ will be found numerically using Matlab. Both Runge-Kutta implementations were very close to the analytic solution found using separation of variables. The infinity norm of the difference between SSPRK and RK4 implementations were calculated to be within 4.2395×10^{-9}. For this reason, Runge-Kutta order 4 was used for any subsequent calculations.

Corrector

We hope to improve upon the linear corrector by using the integral balance equations to produce a nonlinear corrector. To this end, Dr. Cooper wrote a corrector as detailed in [3]. A reliable corrector is still in progress. However, a first version has been implemented. Results of this implementation follow.

Corrector, cont.

Integral Evaluations

To produce a nonlinear corrector, equations (9) and (10) have to be evaluated. From equation (9),

$$T^{\eta}_{(c)}(t,x) = -\frac{M}{L}\int_0^L (\tilde{v}(t,y) - \overline{v}^{\eta}(t,x))^2 \psi_{\eta}(x-y) J(t,y)\ dy,$$

where $\tilde{v}(t,y)$ is the interpolation of the velocity, $\overline{v}^{\eta}(t,x)$ is the average velocity on the mesoscale, $\psi_{\eta}(x-y)$ is the windowing function and $J(t,y)$ is the Jacobian.

Corrector, cont.

Integral Evaluations, cont.

From equation (10):

$$T^{\eta}_{(int)}(t,x) = -\frac{N-1}{N}\int_0^L U'\left(\frac{L}{J(t,y)}\right)\int_0^1 \psi_\eta\left(x-y-\frac{sh}{J(t,y)}\right)\ ds\ dy$$

where U' is the derivative of a potential function.

Corrector, cont.

Integral Evaluations, cont.

In this case we use the Lennard-Jones potential U:

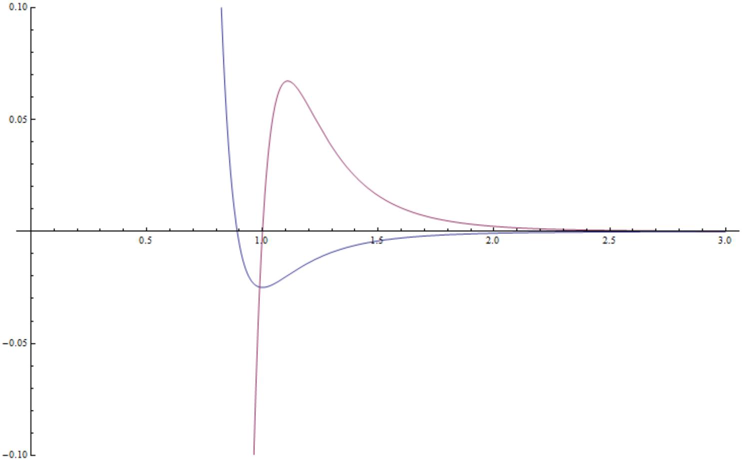
$$U(\xi) = 4\epsilon\left[\left(\frac{\sigma}{\xi}\right)^{12} - \left(\frac{\sigma}{\xi}\right)^{6}\right]$$
$$U'(\xi) = 24\epsilon\left[\left(\frac{\sigma^6}{\xi^7}\right) - \left(\frac{2\sigma^{12}}{\xi^{13}}\right)\right]$$

We may define $\epsilon = 0.25$ as the depth of the potential well, and let $\sigma = 2^{-1/6}$, which is the finite distance at which the potential is zero. ξ is the distance between particles.

Corrector, cont.

Integral Evaluations, cont.

Our Lennard-Jones potential function $U(\xi)$ with $U'(\xi)$:



Corrector, cont.

Integral Evaluations, cont.

We will approximate each using a midpoint approximation

$$\int_a^b f(y)\ dy \approx (\triangle y) \sum_{i=0}^{n-1} f(y_i)$$

where $(\triangle y) = \frac{b-a}{n}$ and $y_i = a + (i + \frac{1}{2})(\triangle y)$.

In order to evaluate these integrals we need to make the following substitutions.

$$\triangle y = \frac{b-a}{n} = \frac{L}{n},$$
$$y_i = \frac{iL}{n},$$
$$J(y_i) = \bar{\rho}^{\eta}.$$

Corrector, cont.

Integral Evaluations, cont.

$T^{\eta}_{(c)}(t,x)$, written independently of t, is

$$\begin{aligned} T^{\eta}_{(c)}(t,x) &= -\frac{M}{L}\int_0^L (\tilde{v}(y) - \overline{v}^{\eta}(x))^2 \psi_{\eta}(x-y)J(y)\ dy \\ &\approx -(\triangle y)\frac{M}{L}\sum_{i=0}^{n-1}(\tilde{v}(y_i) - \overline{v}^{\eta}(x))^2\psi_{\eta}(x-y_i)J(y_i) \\ &\approx -\frac{\overline{\rho}^{\eta}M}{\eta n}\sum_{i=0}^{n-1}(\tilde{v}\left(\frac{iL}{n}\right) - \overline{v}^{\eta}(x))^2\psi\left(\frac{1}{\eta}\left(x-\frac{iL}{n}\right)\right). \end{aligned}$$

Corrector, cont.

Integral Evaluations, cont.

Meanwhile, $T^{\eta}_{(int)}(t,x)$ is a set of two nested integrals.

However, the inner integral can be approximated simply:

$$\begin{aligned}
&\int_0^1 \psi_\eta\left(x-y-\frac{sh}{J(t,y)}\right)\; ds \\
&\approx \frac{h}{2}\left[\psi_\eta\left(x-y-\frac{sh}{J(t,y)}\right)+\psi_\eta\left(x-y\right)\right] \\
&\approx \frac{L}{2\eta N}\left[\psi\left(\frac{1}{\eta}\left(x-y-\frac{L}{N\bar{\rho}^\eta}\right)\right)+\psi\left(\frac{1}{\eta}\left(x-y\right)\right)\right]
\end{aligned}$$

Corrector, cont.

Integral Evaluations, cont.

Note that this is *inside* the outer integral variable dy, and so the interior stress can be evaluated as follows:

$$
\begin{aligned}
&T^{\eta}_{(int)}(t,x) \\
&\approx -\frac{N-1}{N}\int_0^L U'\left(\frac{L}{J(t,y)}\right)\int_0^1 \psi_\eta\left(x-y-\frac{sh}{J(t,y)}\right)\ ds\ dy \\
&\approx -\frac{N-1}{2N}\int_0^L U'\left(\frac{L}{J(t,y)}\right)\left[\psi_\eta(x-y)+\psi_\eta\left(x-y\frac{sh}{J(t,y)}\right)\right]\ dy \\
&\approx -\left(\frac{N-1}{2N}\right)\left(\frac{L^2}{2\eta N^2}\right)U'\left(\frac{L}{\bar{\rho}\eta}\right)\sum_{i=0}^{n-1}\left[\psi\left(\frac{1}{\eta}\left(x-\frac{iL}{n}-\frac{L}{N\bar{\rho}\eta}\right)\right)\right. \\
&\qquad \left.+\,\psi\left(\frac{1}{\eta}\left(x-\frac{iL}{n}\right)\right)\right]
\end{aligned}
$$

Results

- Runge-Kutta Methods for Wave Equation...
- Integral Evaluations...
- Predictor-Corrector Method...

Conclusions

- The nonlinear nature of the mesoscale problem made solving the mesoscale system directly difficult.
- However, the linearization itself provides a good approximation to the microscale problem.
- The predictor-corrector method shows promise as a way of approximating the microscale problem. It is stable in time when a direct approach to solving the nonlinear mesoscale system was not.
- However the corrector itself does not provide a large improvement at this stage. Several attempts have been made to improve the corrector, but work remains to be done.

Thank you!

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