



Direct numerical
simulations of
particle-laden density
with finite-elements

S. D. Parkinson et al.

Direct numerical simulations of particle-laden density currents with adaptive, discontinuous finite elements

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Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Abstract

High resolution direct numerical simulations (DNS) are an important tool for the detailed analysis of turbidity current dynamics. Models that resolve the vertical structure and turbulence of the flow are typically based upon the Navier–Stokes equations. Two-dimensional simulations are known to produce unrealistic cohesive vortices that are not representative of the real three-dimensional physics. The effect of this phenomena is particularly apparent in the later stages of flow propagation. The ideal solution to this problem is to run the simulation in three dimensions but this is computationally expensive.

This paper presents a novel finite-element (FE) DNS turbidity current model that has been built within Fluidity, an open source, general purpose, computational fluid dynamics code. The model is validated through re-creation of a lock release density current at a Grashof number of 5×10^6 in two, and three-dimensions. Validation of the model considers the flow energy budget, sedimentation rate, head speed, wall normal velocity profiles and the final deposit. Conservation of energy in particular is found to be a good metric for measuring mesh performance in capturing the range of dynamics. FE models scale well over many thousands of processors and do not impose restrictions on domain shape, but they are computationally expensive. Use of discontinuous discretisations and adaptive unstructured meshing technologies, which reduce the required element count by approximately two orders of magnitude, results in high resolution DNS models of turbidity currents at a fraction of the cost of traditional FE models. The benefits of this technique will enable simulation of turbidity currents in complex and large domains where DNS modelling was previously unachievable.

GMDD

7, 3219–3264, 2014

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

1 Introduction

Density currents, also known as gravity or buoyancy currents, occur when two fluids with different densities meet. The density difference creates a pressure gradient that causes the more dense fluid to intrude beneath the less dense fluid. They occur in both natural and man-made situations, within a wide range of environments, and over a vast range of temporal and spatial scales. When a fluid contains particles in suspension the bulk density of that fluid changes. Density currents that are at least partly driven by a density variation due to suspended particles are termed particle-laden density currents. Examples include pyroclastic flows, dust storms, avalanches, and turbidity currents.

Submarine particle-laden density currents can occur at a large range of scales (a few m^3 to several 1000's of km^3) and can carry sediment for thousands of kilometres at speeds of up to a hundred kilometres per hour over the sea bed (Heezen and Ewing, 1952; Talling et al., 2007). Turbidity currents, a dilute sub-class of submarine density currents where particle-fluid interactions dominate dynamics, deliver enough destructive power to break telecommunications cables which can have huge financial implications (Heezen and Ewing, 1952). Density currents can have an impact on pollutant dispersal from river outflow (Huang et al., 2005; Bombardelli et al., 2004), industrial discharge (Hallworth and Huppert, 1998; Bonnezaze et al., 1993), oil drilling (Curran et al., 2002) and water-injection dredging (Harris et al., 2002). Density currents are also a key process for the movement of organic material into the depths of the ocean and play an important role in the global carbon cycle. They form a significant component of the stratigraphic record, and their deposits can form hydrocarbon reservoirs (Kneller and Buckee, 2000; Sequeiros et al., 2009). Having a good understanding of density current behaviour can also allow us to predict and improve water quality in reservoirs by enhancing our understanding of pollutant concentrations (Alavian et al., 1992; Huang et al., 2005) and oxygenation (Best et al., 2005).

GMDD

7, 3219–3264, 2014

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Studying sediment-laden currents is not easy. They occur infrequently and unpredictably at any particular location, and tend to destroy any measurement devices that are positioned to measure their effects. The dynamics of these currents are highly complex, with strong feedback between turbulence and sediment suspension making measurement of the dynamics difficult (Kneller and Buckee, 2000; Serchi et al., 2012). Small scale laboratory experiments can provide useful insight into the dynamics of these currents, but are limited by scaling issues and the available measurement techniques (Kneller and Buckee, 2000).

High resolution numerical models have become an important tool for the detailed analysis of particle-laden density current dynamics. Models that resolve the vertical structure of the flow are typically based upon the Navier–Stokes equations. Direct numerical simulations (DNS) of particle-laden density currents should be carried out in three-dimensions as unrealistic cohesive vortices form in two-dimensions that have a significant impact on virtually all of the important outputs from these simulations (Cantero et al., 2007; Espath et al., 2014). DNS modelling of particle-laden density currents has been achieved in three dimensions at moderate Grashof numbers, which approximates the ratio of buoyant to viscous forces, of $\mathcal{O}(10^6)$ by Necker et al. (2002) and Nasr-Azadani and Meiburg (2011). Espath et al. (2014) have simulated a particle-laden density current at a Grashof number of $\mathcal{O}(10^8)$. Computational power has limited modelling of higher Grashof number flows. A Grashof number of $\mathcal{O}(10^8)$ translates to modelling of low particle concentration 10^{-4} – 10^{-3} % flows in water at laboratory scales. Even within this restricted range a lot has been learnt from these models.

There has been some success in modelling these flows using DNS in two dimensions which makes the problem more computationally tractable (Blanchette et al., 2005; Ooi et al., 2007). However, Espath et al. (2014) showed that the only important diagnostic that can be accurately predicted using a two-dimensional DNS model is the sedimentation rate. Another alternative to three-dimensional DNS is to use turbulence models to handle the small scale turbulence and only resolve the large scale motions. Turbulence modelling is undoubtedly important for extending models that resolve the vertical

structure of the flow to more realistic Grashof numbers. Whether it is appropriate to use a turbulence model depends upon the diagnostics that are important in the study. DNS simulations are necessary to perform detailed analysis of turbulent structures, and also for the validation of turbulence models for this application.

This paper presents a novel finite-element (FE) particle-laden density current model that has been built within Fluidity, an open source, general purpose, multiphase computational fluid dynamics code (Pain and Piggott, 2013). The model utilises adaptive meshing technologies to produce high resolution DNS models of particle-laden density currents in three dimensions, at a fraction of the cost of traditional FE models. This paper details validation through recreation of a lock release density current at a Grashof number of 5×10^6 in two and three dimensions. It is shown that adaptivity reduces the required element count by approximately two orders of magnitude for this application. The computational savings afforded by this, along with the flexibility of FE discretisations mean that the model offers many opportunities to investigate particle-laden density current dynamics in complex and large domains.

2 Mathematical model

2.1 Governing equations

A general discussion of particle motion in a non-uniform flow by Maxey and Riley (1983) stated that pressure gradient, added mass, viscous Stokes and augmented drag, and buoyancy forces need to be considered. This work considers flows where the particles are very small in relation to the length scales of motion. It also considers situations where the particle density is significantly larger than that of the surrounding fluid. For example, silica is ≈ 2.6 times the density of water in turbidity currents, and ≈ 2600 times the density of air in dust storms. Based upon these restrictions Maxey and Riley (1983) showed that the dominant forces in the equations of motion for a single particle relative to the fluid in which it is suspended are the viscous Stokes drag and buoyancy terms.

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Particle-laden density currents consist of a collection of particles and hence particle collisions must also be considered. The effect of these collisions can be safely ignored by limiting the model to applications where the sediment volume fraction is less than 1% (Necker et al., 2002). Flocculation of sediment particles can be ignored if the model is further restricted to sediment sizes of sand and larger ($> 64 \mu\text{m}$) (Maerz et al., 2011).

Cantero et al. (2008) showed that the effects of inertia on particle motion in density currents are insignificant for particles smaller than $250 \mu\text{m}$ in diameter and hence the model is restricted to sediment diameters below $250 \mu\text{m}$.

Taking all of the above into account the acceleration of particles will be the same as that of the containing fluid. Particles will move with a velocity equal to the sum of the fluid velocity, $\tilde{\mathbf{u}}$, and a settling velocity, $\tilde{u}_s \mathbf{k}$, where $\tilde{}$ denotes a dimensional value. The settling speed, \tilde{u}_s , is obtained by balancing the Stokes drag and buoyancy forces, and $\mathbf{k} = (0, 0, 1)^T$. This means that the evolution of the particle volume fraction, \tilde{c} , can be described with a transport equation of the form

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} + (\tilde{\mathbf{u}}_i - \tilde{u}_s \mathbf{k}_i) \frac{\partial \tilde{c}}{\partial \tilde{x}_i} = \tilde{\kappa} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}_i^2}, \quad (1)$$

where $\tilde{\kappa}$ is the particle concentration diffusivity. Particle concentrations will never be completely uniform. Individual particles will have a range of masses and settling velocities which lead to slight variations in speed and trajectory. As particles move past one-another they interact and cause a self-induced hydrodynamic diffusion (Davis and Hassen, 1988). The magnitude of this diffusivity is generally chosen to be between 0.7–1.0 times the ambient fluid viscosity (Necker et al., 2002; Cantero et al., 2008). Higher values help convergence and stability of the solution. It has been shown that this value has little effect on the relevant flow quantities so long as it does not significantly exceed the ambient fluid viscosity (Hartel et al., 2000).

Calculation of the settling velocity for a sediment particle requires an estimate of the drag force. This is a function of the particle size, density, and shape. Angular grains will have a different drag force to a perfectly spherical grain, which will follow Stokes'

law. Several equations have been developed for estimating the settling velocity of particles empirically, such as those by Dietrich (1982) and Ferguson and Church (2004), all with similar results. Values in this work are non-dimensionalised. Particle size and density are not prescribed with an arbitrarily sized gravity current of a particular Grashof number, and hence choice of a particular equation is irrelevant.

Continuity and momentum balance in this model is governed by the Navier–Stokes equations. The fluid is assumed to be incompressible and, due to the very low volumetric concentrations, the displacement effect of the entrained particles can be ignored. Therefore the velocity field is divergence free. The Boussinesq approximation is adopted, where density is considered constant except in the buoyancy term. The isotropic kinematic viscosity, $\tilde{\nu}$, is assumed constant throughout the model. This leads to the following form for the Navier–Stokes equations

$$\frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} - \tilde{g}' k_i + \frac{\partial}{\partial \tilde{x}_j} \tilde{\mathbf{S}}_{ij}, \quad (2a)$$

$$\frac{\partial \tilde{u}_i}{\partial \tilde{x}_i} = 0. \quad (2b)$$

The stress tensor, $\tilde{\mathbf{S}}$, for an incompressible flow is defined as

$$\tilde{\mathbf{S}}_{ij} = \tilde{\nu} \left(\frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} + \frac{\partial \tilde{u}_j}{\partial \tilde{x}_i} \right), \quad (3)$$

where the buoyancy density, \tilde{g}' , is a function of the sediment density, ρ_c , the ambient fluid density, ρ_a , the magnitude of the acceleration due to gravity, \tilde{g} , and the volumetric concentration of sediment, \tilde{c}

$$\tilde{g}' = \frac{\tilde{\rho}_c - \tilde{\rho}_a}{\tilde{\rho}_a} \tilde{g} \tilde{c}. \quad (4)$$

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



The assumption $\tilde{c} \ll 1$ and $(\tilde{\rho}_c - \tilde{\rho}_a)/\tilde{\rho}_a = \mathcal{O}(1)$ justify the use of the Boussinesq approximation.

Particle-laden density currents deposit and/or erode the surface over which they travel. This means that the suspended mass changes with time i.e. they are non-conservative. They have the potential to accelerate if their mass increases, or decelerate more rapidly due to settling out of the suspended sediment. The dynamics of sediment erosion, or entrainment, are complex. Sediment on the bed will affect turbulence in the boundary layer. Larger sediment grains will shield smaller ones and grains may adhere to each other in the bed. The bed shape will also change as sediment is eroded which would generate complex topography that may promote or inhibit further sediment erosion. Empirical algorithms have been developed for predicting entrainment rates based upon particle parameters and the bed shear stress. Erodible boundaries, Γ^d , are modelled here as a flux boundary condition

$$\mathbf{n}_i \tilde{\kappa} \frac{\partial \tilde{c}}{\partial \tilde{x}_i} = \tilde{u}_s \tilde{E} \text{ on } \Gamma^d, \quad (5)$$

where \tilde{E} is the non-dimensional entrainment rate of sediment into suspension, \mathbf{n} is the boundary unit normal vector.

Garcia and Parker (1991) reviewed empirical formulae by Fukushima et al. (1985); Akiyama and Stefan (1985) and Parker et al. (1986) for predicting the entrainment of non-cohesive sediment in finite size ranges. They validated these against laboratory results, and produced an improved formula for sediment re-entrainment. This has been successfully used in work by Huang et al. (2007) and Sequeiros et al. (2009) when modelling sediment-laden density currents:

$$\tilde{E} = \frac{AZ^5}{1 + AZ^5/0.3}, \quad (6a)$$

GMDD

7, 3219–3264, 2014

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

$$\tilde{Z} = \frac{\sqrt{\tilde{\tau}_b}}{\tilde{u}_s} \left(\sqrt{\left(\frac{\tilde{\rho}_c - \tilde{\rho}_a}{\tilde{\rho}_a} \tilde{g} \tilde{d} \right) \frac{\tilde{d}}{\tilde{v}}} \right)^{0.6}, \quad (6b)$$

where $A = 1.3 \times 10^{-7}$ is a non-dimensional constant and \tilde{d} is the diameter of the suspended sediment. The bed shear stress, $\tilde{\tau}_b$, is defined as

$$\tilde{\tau}_b = \left| \mathbf{n}_i \tilde{\mathbf{S}}_{ij} \right|. \quad (7)$$

The total flux through an erodible boundary is calculated as:

$$\frac{\partial \tilde{\eta}}{\partial \tilde{t}} = \mathbf{n}_i \tilde{u}_s \mathbf{k}_i \tilde{c}_b - \tilde{u}_s \tilde{E}, \quad (8)$$

where $\tilde{\eta}$ is the volume of the sediment in the bed and \tilde{c}_b is the volumetric concentration of sediment at the sediment bed boundary. \tilde{E} is limited such that it never exceeds $\tilde{\eta}/\Delta t$, where Δt is the period of a time step.

It is also possible for sediment to be moved along the bed without being entrained into the flow. This process is known as bedload transport. This has not been included in the current work. Sequeiros et al. (2009) stated that suspended sediment is the key factor in the movement of sediment in turbidity current and that bedload transport can be neglected for currents that do not have a significant fraction of particles larger than $100 \mu\text{m}$.

Four parameters are used to non-dimensionalise the equations outlined above.

$$Gr = \left(\frac{\tilde{u}_b \tilde{h}_0}{\tilde{v}} \right)^2, \quad (9)$$

$$Sc = \frac{\tilde{v}}{\tilde{\kappa}}, \quad (10)$$

GMDD

7, 3219–3264, 2014

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



$$u_s = \frac{\tilde{u}_s}{\tilde{u}_b}, \quad (11)$$

$$R_p = \sqrt{\left(\frac{\tilde{\rho}_c - \tilde{\rho}_a}{\tilde{\rho}_a} \tilde{g} \tilde{d}\right) \frac{\tilde{d}}{\tilde{v}}}, \quad (12)$$

where Gr is the Grashof number, Sc is the Schmidt number, R_p is the particle Reynolds number, and h_0 is a characteristic length scale (half the lock-release depth in this work, as defined in Sect. 3). The buoyancy velocity, \tilde{u}_b , is used as the characteristic velocity scale and is defined in terms of the initial buoyancy density, \tilde{g}'_0 , and the characteristic length h_0 , as

$$\tilde{u}_b = \sqrt{\tilde{g}'_0 h_0}. \quad (13)$$

Equations (1–3) and (5–8) can now be redefined as

$$\frac{\partial c}{\partial t} + (\mathbf{u}_i - u_s \mathbf{k}_i) \frac{\partial c}{\partial \mathbf{x}_i} = \frac{1}{\sqrt{Sc^2 Gr}} \frac{\partial^2 c}{\partial \mathbf{x}_i^2}, \quad (14)$$

$$\frac{\partial \mathbf{u}_i}{\partial t} + \mathbf{u}_j \frac{\partial \mathbf{u}_i}{\partial \mathbf{x}_j} = -\frac{\partial p}{\partial \mathbf{x}_i} - \mathbf{k}_i c + \frac{\partial}{\partial \mathbf{x}_j} \mathbf{S}_{ij}, \quad (15)$$

$$\frac{\partial \mathbf{u}_i}{\partial \mathbf{x}_i} = 0, \quad (16)$$

$$\mathbf{n}_i \frac{1}{\sqrt{Sc^2 Gr}} \frac{\partial c}{\partial \mathbf{x}_i} = u_s E \quad \text{on } \Gamma^d, \quad (17)$$

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



$$E = \frac{A Z^5}{1 + A Z^5/0.3}, \quad (18)$$

$$Z = \frac{\sqrt{\tau_b}}{u_s} R_p^{0.6}, \quad (19)$$

$$\tau_b = |\mathbf{n}_i \mathbf{S}_{ij}|, \quad (20)$$

$$\frac{\partial \eta}{\partial t} = \mathbf{n}_i u_s \mathbf{k}_i c_b - u_s E, \quad (21)$$

$$\mathbf{S}_{ij} = \frac{1}{\sqrt{Gr}} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \quad (22)$$

2.2 Discretisation

Fluidity uses the finite element method to solve the Navier–Stokes equations. Using finite elements gives great flexibility in element choices and many are available when using Fluidity. A linear Discontinuous Galerkin (DG) scheme is used for the discretisation of both the velocity and sediment concentration fields. DG methods are a good choice of discretisation for advection-dominated problems as they produce stable discretisations without the need for stabilisation strategies such as streamline-upwinding (Peraire and Persson, 2008). DG methods also work well on arbitrary meshes and have the desirable properties of having a block diagonal mass matrix that can be trivially inverted locally for each element. This allows for certain equations to be solved very cheaply (Bassi and Rebay, 1997).

Use of the DG method requires a choice of flux schemes for both the advective and diffusive terms. A simple upwind flux is chosen for advective terms. A centred flux is used for the diffusive terms. The compact discontinuous Galerkin method (CDG)

is used to implement the diffusive terms (Peraire and Persson, 2008). For a detailed discussion of DG discretisations and flux terms see the review paper by Cockburn and Shu (2001).

Advection when using a DG discretisation is not bounded. Undershoots and overshoots can occur that affect the dynamics of a gravity current. Slope limiters are employed to bound the solution although these can be dissipative. Vertex-based slope limiting, as suggested by Kuzmin (2010), is used herein.

For the pressure field a quadratic Continuous–Galerkin scheme is used. We therefore have a mixed finite element pairing for solving the incompressible Navier Stokes equations. This element pairing, described by Cotter et al. (2009), has the benefit of satisfying the Ladyženskaja–Babuška–Brezzi (LBB) stability condition and hence needs no stabilisation of the pressure field. Additionally, a higher order accurate pressure field means that the pressure gradient term in the momentum equation is the same order accuracy as the buoyancy forcing term. These two terms dominate in early stages of propagation and hence the ability for these terms to balance is important in determining how the flow evolves.

A Crank–Nicolson time discretisation is used throughout the model which is second-order accurate in time. The coupled system of non-linear equations are solved using two non-linear iterations known as Picard iterations. Within each non-linear iteration the equations are linearised using the best available solution for each variable that is not being solved for. The momentum and conservation equations are solved using a pressure correction scheme.

There are two exceptions to the use of Crank–Nicolson time discretisation. Slope limiters used with DG discretisations only guarantee a bounded solution in conjunction with an explicit advection scheme. Therefore the sediment transport and momentum equations are solved in two stages. Advection is calculated using 10 explicit subcycles with time steps of $\Delta t/10$, then diffusion/viscous dissipation occurs with Crank–Nicolson discretisation. Additionally, the bed shear stress is calculated at the start of each time

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

step and hence the re-entrainment rate is totally explicit. Full details of the time discretisation outlined above are available in the Fluidity manual (Pain and Piggott, 2013).

An adaptive time step is used. This makes the simulation more robust when using a changing mesh and also takes advantage of the reducing current velocity over time which allows for much larger time steps towards the end of the simulation. The time step length is based upon obtaining a target Courant number of 2.0. This is a relatively conservative requirement for the implicit time discretisation used.

2.3 Anisotropic mesh adaptivity

The motivation behind using mesh adaptivity is to optimise the spatial resolution with time such that both the discretisation error and computational cost of a simulation are minimised (Piggott et al., 2005). Adapting the mesh is split into three tasks. The first step is to determine the desired edge lengths, or to form a metric against which element edge lengths can be defined, the second part involves generating a new mesh that better fits these requirements and distributing this mesh amongst the active processors, and the third involves transferring data from the old mesh to the new mesh.

2.3.1 Metric formation

Determining the desired edge lengths for a mesh requires some quantification of the error in the solution due to spatial discretisation. This is difficult to do as there is usually no better estimate of the exact solution than the estimate from the current discretisation. An indirect method of measuring the error is required. Ciarlet (1991) showed that the finite element error can be bounded by the interpolation error for elliptic problems. It is assumed that this also holds for other partial-differential equations. This is a reasonable way of defining an error estimate (Fortin, 2000).

The aim is to minimise the error in fields that are discretised using first order discretisations. For first order elements, the interpolation error depends upon the Hessian, \mathbf{H} (the matrix of second-order partial derivatives) (Frey and Alauzet, 2005). The

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

second derivative of such a discretisation is formally zero and hence some method of recovering the Hessian for these fields is needed. In Fluidity a double lumped Galerkin projection is used to compute the Hessian as described by Pain et al. (2001). This Hessian will contain information about both the magnitude and direction of the curvature of a field and hence can be used to guide generation of anisotropic elements. This is very useful in regions, such as boundary layers, where the solutions vary significantly more rapidly in one direction than in others.

The Hessian is used to form a metric tensor, \mathbf{M} , that will guide the mesh optimisation. \mathbf{M} is defined such that the optimal mesh, \mathcal{M} , would have edges, \mathbf{v} , with unit length when measured against it

$$\sqrt{\mathbf{v}_i \mathbf{M}_{ij} \mathbf{v}_j} = 1 \quad \forall \mathbf{v} \in \mathcal{M}. \quad (23)$$

The choice of formulation for \mathbf{M} is therefore fundamental to the way in which the mesh adapts. A formulation suggested by Chen et al. (2007) which controls the L^2 norm of the interpolation error is used

$$\mathbf{M} = \frac{1}{\varepsilon} \det|\mathbf{H}|^{-\frac{1}{4+n}} |\mathbf{H}|, \quad (24)$$

where n is the number of dimensions, and ε is the interpolation error bound, a value which is defined by the user. For L^p methods, Loseille and Alauzet (2011) found $p = 2$ to be the optimal value and incorporate more influence from dynamics of smaller magnitudes. Experience has shown this metric formation to be very effective for gravity current simulations (Hiester et al., 2011, 2014).

It is often important to adapt to more than one solution field. When this is the case the final metric is a superposition of the metrics calculated for each individual field (Pain et al., 2001). At this point the metric is also modified to take into account bounds upon the maximum and minimum element size, maximum allowable aspect ratio, edge length gradation, and the number of elements. Additionally, this metric can be advected forward in time providing an estimate of future requirements for the mesh resolution and allowing for more time between adapt operations (Hiester et al., 2011).

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

As such the experiment configuration is identical to that of Necker et al. (2002), with the exception of the addition of sediment erosion, and hence a requirement for the definition of R_p . R_p is defined to lie in the range of R_p for which the erosion algorithm outlined in Eq. (18) is valid, as detailed in Garcia and Parker (1991).

Boundary conditions for velocity are free-slip for all side walls, $\mathbf{u}_1 = 0.0$ at $x = -1.0$ and $x = 18.0$, $\mathbf{u}_2 = 0.0$ at $y = 0.0$, and $y = 2.0$, and no-slip at the top and bottom of the domain, $\mathbf{u} = (0.0, 0.0, 0.0)^T$ at $z = 0.0$ and $z = 2.0$. All velocity boundary conditions are applied weakly. Where a velocity component is not set with a Dirichlet condition, a zero Neumann boundary condition is applied. Note that the side wall boundary conditions vary from those of Necker et al. (2002). A free slip boundary condition will give comparable results to the periodic boundary conditions used in that work.

Boundary conditions for the sediment concentration field are as follows. The erosion boundary condition outlined in Eq. (17) is applied at the bottom surface, $z = 0.0$. A zero Dirichlet boundary condition is prescribed at $z = 2.0$ (the top surface of the tank). At all other boundaries $(\mathbf{u} + k\mathbf{u}_s) \cdot \mathbf{n}$ equals zero, hence zero Neumann boundary conditions are applied which enforce zero flux of sediment across these surfaces.

The initial condition for the sediment concentration field in the three-dimensional simulation is similar to that suggested by Hartel et al. (1997) and Cantero et al. (2006). This initial condition is based upon the solution obtained from a purely diffusive problem. Hartel et al. (1997) argued that the problem will be dominated by diffusion for very early stages of the simulation and hence this initial condition is justified as being the condition of the flow a short time period after the initial release. This initial condition includes a perturbation, γ , in a similar way to the work by Cantero et al. (2006). A random perturbation of the initial condition is important to help promote the generation of three-dimensional structures in the flow. Necker et al. (2002) and Espath et al. (2014) use an alternative perturbation of the velocity field for the same purpose. The initial condition for the sediment concentration, including the perturbation, is as follows

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

$$c = \frac{1}{2} - \frac{1}{2} \operatorname{erf} \left\{ \sqrt[4]{GrSc^2} [x - \gamma] \right\}, \quad (26)$$

with

$$\gamma = \cos \left(\sum_i f(i, x, y, z) \right) \Delta_x, \quad (27)$$

where Δ_x is chosen to be 0.2. γ is constructed of four sets of waves originating from the four corners of a plane aligned with the lock gate. Each set of waves contain 60 waves with random phases and random wavelengths ranging between 0.02 and ∞ . Wave i has amplitude $f(i, x, y, z)$ at positions x, y, z . The perturbation chosen covers a wide range of frequencies so as to not preferentially generate particular wavelengths of oscillations. The mesh is adapted before the first time step to produce a good mesh for this initial condition.

To use adaptivity several controlling parameters need to be defined. The fundamental parameters which define the mesh resolution in the simulation are the interpolation error bounds. The next section describes how values for these parameters were chosen. The time between adapts also requires definitions, and it is necessary to ensure that there is adequate resolution in periods between adapts. Through experimentation it was found that an adapt every 5 time steps kept the simulation stable towards the beginning of the simulation. At later stages in the simulation an adapt was required every 2 time steps. The high frequency of mesh adapts was required to limit instabilities in the boundary layer which grow rapidly. Small instabilities that developed did not have any noticeable impact on the important outputs from the simulation. This is discussed further in the following sections. As mentioned in Sect. 2.3.1, metric advection is used to advect the metric, which defines the edge lengths required to meet the interpolation error bounds, forward in time. The metric is conservatively advected through 5 adapt intervals at each adapt.

4 Choosing appropriate interpolation error bounds

It is possible to define an interpolation error bound for any of the functions in the simulation. In this simulation sediment concentration, velocity, and pressure are solved for. It is common practice to adapt to the velocity field for the purposes of resolving the velocity and pressure fields. Good resolution of the sediment concentration field is also required. Hence four interpolation error bounds require definition for the simulation, one for each velocity component, and another for the sediment concentration.

In order to select good values for these parameters a convergence analysis is required. Doing this with three-dimensional models would be prohibitively expensive and hence two-dimensional simulations are used to carry out this convergence analysis. The two-dimensional simulations are defined in the $x - z$ plane. It has been well documented by Necker et al. (2002) and Cantero et al. (2007) that output from two-dimensional simulations of particle-laden density currents do not compare well with three-dimensional simulations. However, two-dimensional simulations are useful for the purpose of understanding the resolution requirements of simulations.

A measure of the quality of a mesh, in terms of the dynamics computed within it, is required. The simulation is of a turbulent flow. Head speed, deposit profile, quantity of suspended sediment and deposition rates are all important outputs from these simulations, but due to the turbulent nature of the flow, which is very sensitive to small changes in the mesh, it is very hard to show convergence of these quantities.

However, one important quantity does show convergence. DNS simulations resolve all length scales of motion. Convergence analysis will show that the discretisation errors are small enough that they have a negligible impact on the result and that the mesh resolution is fine enough to resolve all of the energy in the flow. The combination of upwind flux terms and slope limiting in the discretisation dissipates energy at scales that the mesh cannot resolve. Additionally, adapting the mesh requires a data transfer operation which produces errors in conservation of energy, although these are minimal compared to the numerical dissipation from an under-resolved mesh. By computing the

GMDD

7, 3219–3264, 2014

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

energy budget in the simulation and how this varies over time a value for the energy lost due to discretisation, and data transfer errors, ϵ_E can be obtained. This quantity gives us some indication of how well the scales of motion in the flow are being resolved. Importantly, this value converges as the mesh resolution increases and so gives us a good method of comparing the quality of different mesh configurations. Following the method of Winters et al. (1995); Necker et al. (2002) and Espath et al. (2014) after them, equations for the rates of change of potential energy, E_p , and kinetic energy, E_k , in the system can be derived as follows.

The kinetic energy in the system is

$$E_k = \frac{1}{2} \int_{\Omega} |\mathbf{u}|^2 d\Omega. \quad (28)$$

To obtain the time derivative for E_k compute the dot product of the momentum Eq. (15) with \mathbf{u} and apply the chain rule to obtain

$$\frac{1}{2} \frac{\partial |\mathbf{u}|^2}{\partial t} + \frac{1}{2} \mathbf{u}_j \frac{\partial |\mathbf{u}|^2}{\partial x_j} = -\mathbf{u}_i \frac{\partial p}{\partial x_i} - \mathbf{u}_3 c + \mathbf{u}_i \frac{\partial \tau_{ij}}{\partial x_j}. \quad (29)$$

Integrating over the domain and integrating by parts, using the continuity Eq. (16) and the knowledge that there are no normal flow boundary conditions on all boundaries, i.e. $\mathbf{u}_i \mathbf{n}_i = 0$, an equation for the rate of change of E_k is obtained

$$\frac{\partial E_k}{\partial t} = - \int_{\Omega} c \mathbf{u}_3 d\Omega - \int_{\Omega} \tau_{ij} \frac{\partial \mathbf{u}_i}{\partial x_j} d\Omega. \quad (30)$$

The potential energy in the system is

$$E_p = \int_{\Omega} c x_3 d\Omega. \quad (31)$$

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page	
Abstract	Introduction
Conclusions	References
Tables	Figures
⏪	⏩
◀	▶
Back	Close
Full Screen / Esc	
Printer-friendly Version	
Interactive Discussion	



To obtain the time derivative for this term first multiply the equation for sediment concentration (Eq. 14) by x_3

$$\frac{\partial c}{\partial t} x_3 + x_3 (\mathbf{u}_i - u_s \mathbf{k}_i) \frac{\partial c}{\partial x_i} = x_3 \frac{1}{\sqrt{Sc^2 Gr}} \frac{\partial^2 c}{\partial x_i^2}. \quad (32)$$

5 Integrating over the domain, and by parts, using the chain rule and noting that all velocities normal to the wall are zero, an equation for the rate of change of E_p is obtained

$$\frac{\partial E_p}{\partial t} = \int_{\Omega} c \mathbf{u}_3 d\Omega + u_s \int_{\Omega} x_3 \frac{\partial c}{\partial x_3} d\Omega + \frac{1}{\sqrt{Sc^2 Gr}} \left[\int_{\Gamma} x_3 \frac{\partial c}{\partial x_i} \mathbf{n}_i d\sigma - \int_{\Omega} \frac{\partial c}{\partial x_3} d\Omega \right]. \quad (33)$$

10 An equation for the transfer of energy from E_k and E_p to and from internal energy and heat, and also lost due to the settling of particles can be obtained by combining Eqs. (30) and (33). This equation will not hold for an under-resolved mesh. Energy dissipation that occurs at scales below the grid resolution will be dissipated through application of slope limiting. An additional term, ϵ_d , is therefore included to balance the equation and represent the dissipation due to numerical errors.

$$15 \frac{\partial (E_p + E_k)}{\partial t} = -\epsilon - \epsilon_s - \epsilon_d, \quad (34)$$

where

$$\epsilon = \int_{\Omega} \boldsymbol{\tau}_{ij} \frac{\partial \mathbf{u}_j}{\partial x_i} d\Omega, \quad (35)$$

20 and

$$\epsilon_s = \frac{1}{\sqrt{Sc^2 Gr}} \left[\int_{\Omega} \frac{\partial c}{\partial x_3} d\Omega - \int_{\Gamma} x_3 \frac{\partial c}{\partial x_i} \mathbf{n}_i d\sigma \right] - u_s \int_{\Omega} x_3 \frac{\partial c}{\partial x_3} d\Omega. \quad (36)$$

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page	
Abstract	Introduction
Conclusions	References
Tables	Figures
⏪	⏩
◀	▶
Back	Close
Full Screen / Esc	
Printer-friendly Version	
Interactive Discussion	



In order to compare mesh quality ϵ_d is integrated over time to give

$$E_D = \int_0^t |\epsilon_d(\tau)| d\tau. \quad (37)$$

E_D is computed for a set of two-dimensional simulations forming a parameter sweep of values for the interpolation error bounds for the two components of velocity and sediment concentration with values of 4×10^{-3} , $4 \times 10^{-2.5}$ and 4×10^{-2} . This leads to a total of 27 simulations. The range of values used in the parameter sweep were determined from sensitivity analyses performed prior to this. For the purposes of comparing results against fixed mesh simulations the above quantity was also computed for a range of regular, structured triangular mesh simulations with edge-lengths 5×10^{-2} , 2.5×10^{-2} , 1.25×10^{-2} , and 6.25×10^{-3} . The adaptive mesh simulations converge at a higher order than the fixed mesh simulations in relation to the mean number of elements, \bar{N}_e , used in the simulation (Fig. 2). The number of elements in adaptive mesh simulations, N_e , varies with time (Table 1). The difference between the maximum and minimum number of elements increases superlinearly as the interpolation error bounds tighten. The number of elements in the domain is a function of the interpolation error bounds, the dynamics of the flow, which vary significantly with time and also mesh resolution, creating a non-linearity in this relationship, and also the bound set for the maximum element size. The largest relative difference between the maximum and minimum number of elements occurs in adaptive simulation A2 where the maximum is $\approx 130\%$ of the mean, and the minimum is $\approx 40\%$ of the mean. The distribution of element counts throughout a simulation is skewed. An increase in the number of elements implies that element size has decreased. This in turn implies that the length of timesteps has decreased leading to more timesteps being required at periods during which there are a large number of elements.

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Importantly, Fig. 2 shows that, at the highest resolutions, a saving of more than one order of magnitude is obtained in the mean number of elements required in the simulation. In three-dimensions the saving are likely to be even greater.

Integrating Eq. (38) over time

$$E_p + E_k = \int_0^t -\epsilon(\tau) - \epsilon_s(\tau) - \epsilon_d(\tau) d\tau = -E - E_s - E_d. \quad (38)$$

Figure 3 shows how the above quantities vary over the period of the simulation for adaptivity options A3, as detailed in Table 1. Values are compared against two-dimensional results (Espath et al., 2014). There is very good agreement for E , but there is a notable variation between the values for E_s in this work and that of Espath et al. (2014). This is because of the zero Dirichlet boundary condition for sediment concentration at the top of the tank in this work where Espath et al. (2014) has a zero flux condition. At very early stages of the simulation the Dirichlet condition results in a flux of sediment through the top of the domain. The overall impact on the simulation is a loss of sediment mass of $< 1\%$ and a total energy loss of $\approx 3\%$. The zero flux condition is preferable but is not implemented in Fluidity for this discretisation. A future aim will be to implement this boundary condition. Generally there is good agreement for E_k and E_p . In two-dimensional simulations strong coherent vortices form that contain and move large quantities of the suspended sediment. These vortices play an important role in the transfer of energy between E_k and E_p . Because of the chaotic nature of the creation and propagation of the vortices, there will always be variations in the values of E_k , E_p and to some extent E between simulations.

Another important aspect of the flow is the boundary layer at no-slip boundaries. This feature of the flow requires very small elements in the wall normal direction to resolve the boundary layer properly. Convergence on a solution is quickly obtained for the boundary layer using an adaptive mesh (Fig. 4). All but the most coarse adaptive simulation configurations have converged on to a solution. The fixed mesh

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page	
Abstract	Introduction
Conclusions	References
Tables	Figures
⏪	⏩
◀	▶
Back	Close
Full Screen / Esc	
Printer-friendly Version	
Interactive Discussion	



configurations show a similar level of convergence for the two highest resolution simulations. Anisotropic mesh adaptivity is particularly useful for resolving features such as boundary layers which require high resolution in one direction compared to others.

Using the evidence outlined above, the chosen interpolation error bounds were those of adaptive simulation A3. This simulation had a well resolved boundary layer and good conservation of energy. This simulation had interpolation error bounds of $4 \times 10^{-2.5}$ for both velocity components. An assumption is made that this error bound will also be suitable for the third velocity dimension in the three-dimensional simulation.

Figure 5 shows a qualitative comparison of results from high and low resolution fixed mesh simulations, and an adaptive mesh simulation, A3. The low resolution fixed mesh simulation has approximately the same number of elements as the adaptive simulation but is clearly not resolving the turbulent structures as well as the adaptive mesh simulation. Results from the high resolution fixed mesh and the adaptive mesh simulations are very similar. There are some variations in the vortices that are generated and these variations grow with time. Within the scope of this investigation no two simulations ever produced identical results. Very small variations in spatial discretisation lead to small variations at early stages in the simulation which propagate and lead on to larger variations downstream.

5 The benefits of using adaptivity

In three-dimensions, adaptivity is essential to compute this simulation using finite elements with Fluidity. A fixed, and regular tetrahedral grid would have required more than 1×10^9 elements which would have led to an unachievable run time and unmanageable post-processing and visualisation demands. By using adaptivity the number of required elements has been reduced to a maximum of approximately 1×10^7 , at least a two order of magnitude reduction, making all aspects of the simulation manageable.

Figure 6 shows how the number of elements in the simulations varied over time. Throughout the simulation the number of processor cores that were used was varied

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

between 36 and 512 to keep the number of elements per core in the region of 20000. The initial drop in number of elements at the start of the simulation is due to the fact that conservative interpolation bounds were used to generate the mesh from the initial conditions. Following this initial drop, during early periods of the simulation the flow is transitioning from a laminar to a turbulent flow. Throughout this period u becomes more and more complex and hence the number of elements required to resolve the flow increase rapidly. The highest amount of elements required is at a $t \approx 10$ at which point the flow has developed into a fully three-dimensional, highly turbulent flow. Beyond this point the number of elements required for the simulation steadily decreases as energy is dissipated from the flow. Additionally, c gradually diffuses such that the curvature of the field decreases and fewer elements are required to resolve the field. Note the drop in elements at $t \approx 25$ of approximately 12.5%. This coincides with the reduction in time between adapts from 5 to 2 as mentioned in Sect. 3. A reduction in adapt interval means that the metric is not advected so far, and hence fewer elements are required. Also note the noise in the number of elements in the simulation. This is reduced by adapting more regularly and is due to the adapt routine responding to small instabilities in the boundary layer. Future work will look into removing these instabilities. This may require mesh adapts after every time step.

Figure 7 shows the distribution of element sizes across a plane of the domain at $y = 1.0$ at times $t = 8$ and $t = 20$. Three images for each time show the dimensions of the elements in the x , y , and z directions. High resolution in the z , or wall normal direction, can be seen on no-slip boundaries in proximity to the wall. Much larger relative resolutions are found in the same regions for the x and y directions. This is enabled by the use of anisotropic mesh adaptivity which keeps the number of elements to a minimum, whilst still resolving this important feature of the flow. These images also highlight the cost of resolving the wall boundary layer with a high density of small elements, and hence a large proportion of the elements found in the near wall region. The high wall resolution in the z direction is present on all no-slip surfaces and extends beyond the front of the gravity current head. In the x direction the highest resolution is generally

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

found at the front of the gravity current head. This is caused by a sharp interface in c at the front of the head. There is also high resolution around vortices and at the left hand wall where there is a strong recirculation of the overlying fluid. In the y direction the largest region of high resolution is in the gravity current body just behind the head of the current due to recirculating flow in this region and hence high curvature in c and \mathbf{u}_2 . The distribution of element sizes in this region varies rapidly due to the three-dimensional turbulent structure of the flow. There is a large difference in the resolution between $t = 8$ and $t = 20$. Within the current the resolution has generally decreased by $t = 20$ but a significantly larger proportion of the domain is below the maximum element size. Generally, the elements appear to be smaller in the z direction. This implies that the interpolation error bound may be proportionally tighter on \mathbf{u} in this direction, and could be reduced a little to bring the resolution in line with the other directions.

In Sect. 4 it was shown that an adaptive simulation with the interpolation error bounds used here compared well with the finest fixed mesh simulation (1.25×10^{-2}). It is no surprise that, in the most computationally demanding regions of the flow, Fig. 7 shows that the smallest element edge lengths in the adaptive simulation match well with the fixed mesh edge length.

Adaptivity does come at a cost. The mean time required for an parallel adapt operation throughout this simulation, including mesh adaptation, data-transfer, mesh partitioning and data-migration, was 110 s. This can be compared to a mean time required to compute a time step in parallel of 67 s. Therefore, when adapting every 5 time steps, approximately 1/4 of the simulation time is spent adapting the mesh, or the run time is increased by 33% compared to a fixed mesh simulation using the same number of elements. When adapting every 2 time steps approximately 2/3 of the simulation is spent in the adapt stage. However, the benefits of reducing the number of elements by two orders of magnitude far outweigh this cost. Using adaptivity, the total computing time was approximately 100 000 h of processor time. Over 500 cores this equates to just under a week of run time. Assuming a linear increase in run time with number of

elements, a fixed mesh simulation would have taken at least an order of magnitude longer and would have been nearly impossible to post-process.

The run time of a simulation is dependent upon many parameters. This run time includes the time required for many online diagnostics and the writing of data to disk.

5 When using adaptivity the frequency of adapts is an additional key parameter that governs a trade-off between total processing time and time to completion. Increasing the time between adapts requires a larger amount of elements to ensure that there is adequate resolution throughout the period between adapts. This will increase the total processing time required to solve the problem. However, with more elements,
10 the problem can be split amongst more cores whilst keeping the minimum number of elements per core constant. The time to completion is then likely to reduce as fewer adapt operations are required. This parameter can be varied dependent upon what is important to the scientist. Size of output, time to completion, the cost of processor time, and the size of available computers must all be taken in to account. Another
15 adaptive simulation with similar properties, but slightly varied parameters, could require significantly more, or less total processing hours.

6 Results

Figure 8 shows how the density current propagates along the tank. The perturbation in the initial condition for the concentration field is shown in the image relating to $t = 0$.
20 This initial condition creates the initial three-dimensional instabilities required to generate a realistic density current. By $t = 8$ this flow is fully turbulent and three-dimensional. This is in agreement with other models (Necker et al., 2002; Espath et al., 2014). The well known structures of lobes and clefts are present at the front of the density current from this point onward.

25 Figure 9 shows how the head position varies with time throughout the simulation. This is computed as the maximum x value, averaged across the width of the domain, obtained from a sediment concentration contour at $c = 0.01$. Lines are plotted showing

GMDD

7, 3219–3264, 2014

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



the agreement with other models. The results compare well with Espath et al. (2014), whose model predicted a head position slightly in front of the model by Necker et al. (2002). The addition of erosion of the bottom surface in this simulation will increase the concentration of the head of the flow and may lead to a faster head speed. The same simulation would need to be run without erosion to know whether this is the case. Espath et al. (2014) noted the importance of the initial condition to the development of the flow. The initial conditions used in this work are slightly different to those of Espath et al. (2014) and Necker et al. (2002) and hence complete agreement is not expected.

Figure 10 shows the spatially integrated deposition rates over the course of the simulation. Again the deposition rate shows good agreement with other published values. As noted by Necker et al. (2002) the deposition rate increases at a rate proportional to $t^{0.5}$ until approximately $t = 14$, at which point there is a sharp change and the deposition rate begins to drop rapidly at a rate proportional to $t^{-2.5}$. The key difference between the results from this work and those of the other models is the presence of erosion in this simulation. The deposition rates from this simulation are higher than those of Necker et al. (2002) and Espath et al. (2014). Noting that the vertical fluid velocities are small near the bed due to the no slip boundary condition, and that eroded sediment will be settling, the majority of eroded sediment will almost immediately be deposited, and will never be fully entrained back into the flow. Figure 10 shows a modified deposition rate from the simulation which removes the effect of erosion, assuming that all eroded sediment is immediately deposited. This modified deposition rate brings the results into better agreement with the results of both Necker et al. (2002) and Espath et al. (2014). In good agreement with Espath et al. (2014) a small peak in deposition rate at $t = 4$ is observed.

An important diagnostic for applications is the final deposit profile from a particle-laden density current. Figure 11 shows the span-wise averaged deposit profile from the three-dimensional simulation against those of previous modellers and also from the experiments of De Rooij and Dalziel (2009). A good match is observed in the peak deposit height of $\eta \approx 0.12$ at $x_1 \approx 4$. There are some differences in the results. Notably

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



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Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

- Cantero, M., Balachandar, S., Garcia, M., and Ferry, J.: Direct numerical simulations of planar and cylindrical density currents, *J. App. Mech.*, 73, 923–930, doi:10.1115/1.2173671, 2006. 3234, 3235
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Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

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Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

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Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

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Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Table 1. Minimum, maximum, and mean number of elements for selected adaptive two-dimensional simulations from the interpolation error bound parameter sweep.

id	ε_c	ε_{u_1}	ε_{u_2}	$\min(N_e)$	$\max(N_e)$	\bar{N}_e
A0	$4 \times 10^{-2.0}$	$4 \times 10^{-2.0}$	$4 \times 10^{-2.0}$	12 924	15 000	14 017
A1	$4 \times 10^{-2.5}$	$4 \times 10^{-2.5}$	$4 \times 10^{-2.5}$	16 025	31 083	24 900
A2	$4 \times 10^{-3.0}$	$4 \times 10^{-3.0}$	$4 \times 10^{-3.0}$	20 515	71 055	55 031
A3	$4 \times 10^{-3.0}$	$4 \times 10^{-2.5}$	$4 \times 10^{-2.5}$	19 094	63 767	41 827

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

**Direct numerical
simulations of
particle-laden density
with finite-elements**

S. D. Parkinson et al.

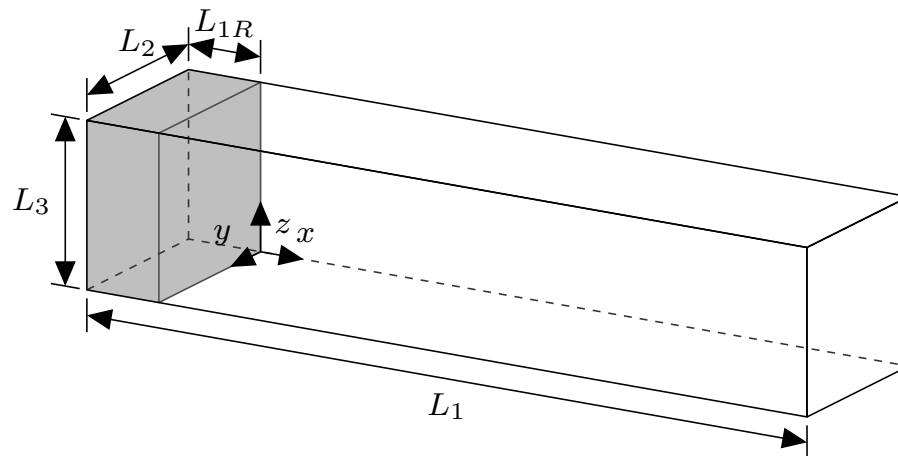


Fig. 1. Lock-release simulation domain configuration. The grey region indicates the volume of non-zero sediment concentration at $t = 0$. The coordinate system defines the origin, x_0 , y_0 , z_0

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

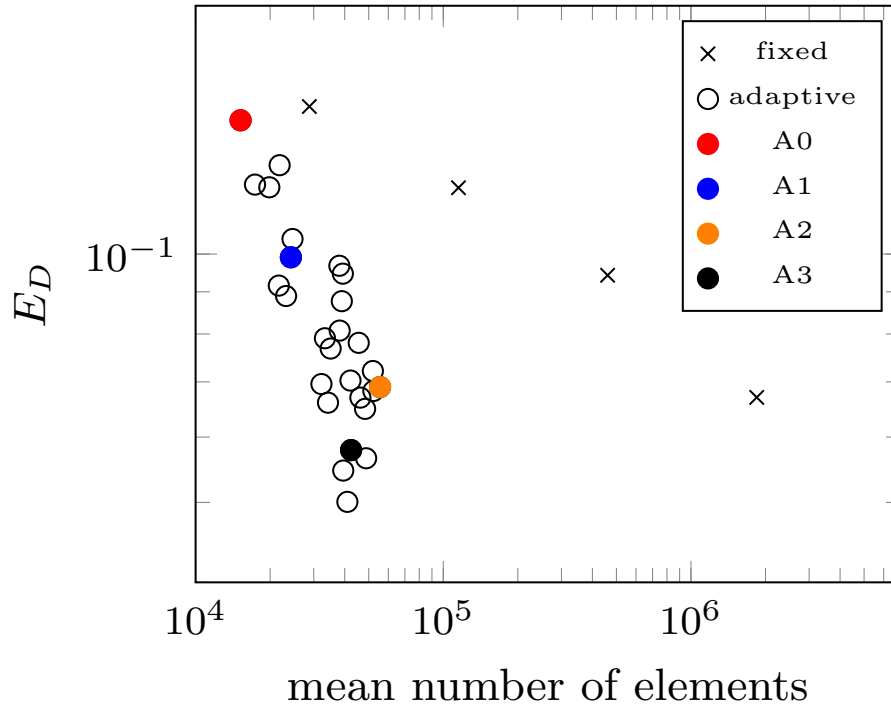


Fig. 2. E_D against the mean number of elements for a range of two-dimensional simulations using fixed and adaptive meshes. Adaptive simulations represent a parameter sweep of interpolation error bounds with values 4×10^{-3} , $4 \times 10^{-2.5}$ and 4×10^{-2} for velocity and concentration. Fixed meshes are on uniform triangular grids with edge-lengths 5×10^{-2} , 2.5×10^{-2} , 1.25×10^{-2} , and 6.25×10^{-3} . Four adaptive simulations are highlighted. The settings for these simulations are detailed in Table 1.

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

⏪ ⏩

◀ ▶

Back Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



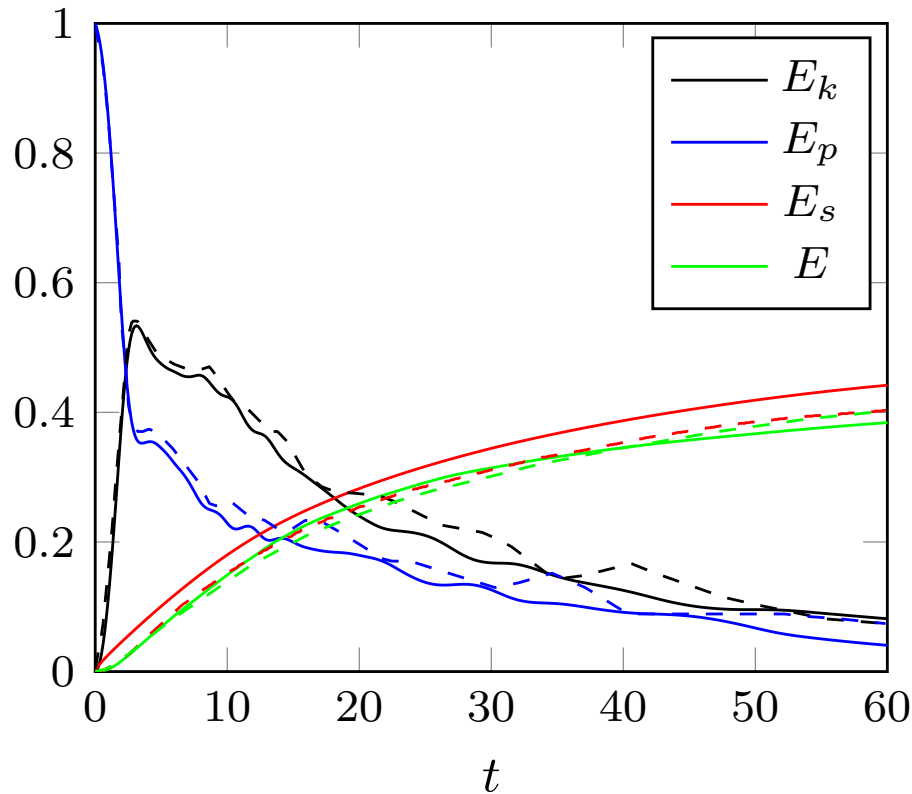


Fig. 3. Energy budget evolution with time for simulation with adaptivity options A3 (solid lines —) compared against 2-D results from Espath et al. (2014) (dashed lines - - -). Values are normalised by the initial potential energy, E_T .

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page

Abstract Introduction

Conclusions References

Tables Figures

⏪ ⏩

◀ ▶

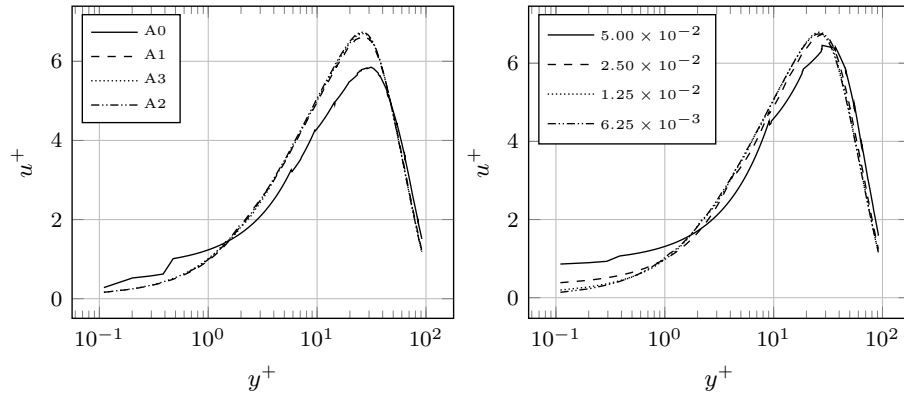
Back Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion





(a) Selected adaptive mesh simulations. (b) Fixed mesh simulations. Legend indicates element edge lengths.

Fig. 4. Wall normal velocity profile at the location of the nose of the gravity current at $t = 7.5$ for the fixed mesh simulations and selected adaptive simulations. Note that A2 is a higher resolution simulation than A3.

Title Page	
Abstract	Introduction
Conclusions	References
Tables	Figures
◀	▶
◀	▶
Back	Close
Full Screen / Esc	
Printer-friendly Version	
Interactive Discussion	

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

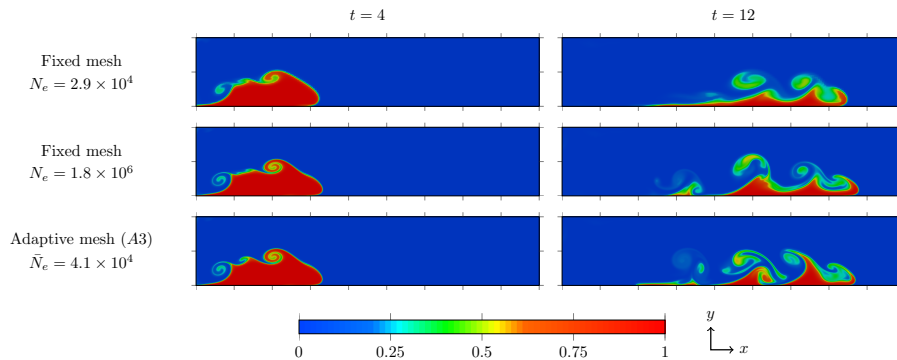


Fig. 5. Heat map of sediment concentration at $t = 4$ and $t = 12$ for the highest resolution fixed mesh simulation the adaptive simulation with configuration A3, and a fixed mesh simulation with a similar number of elements to the adaptive simulation.

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



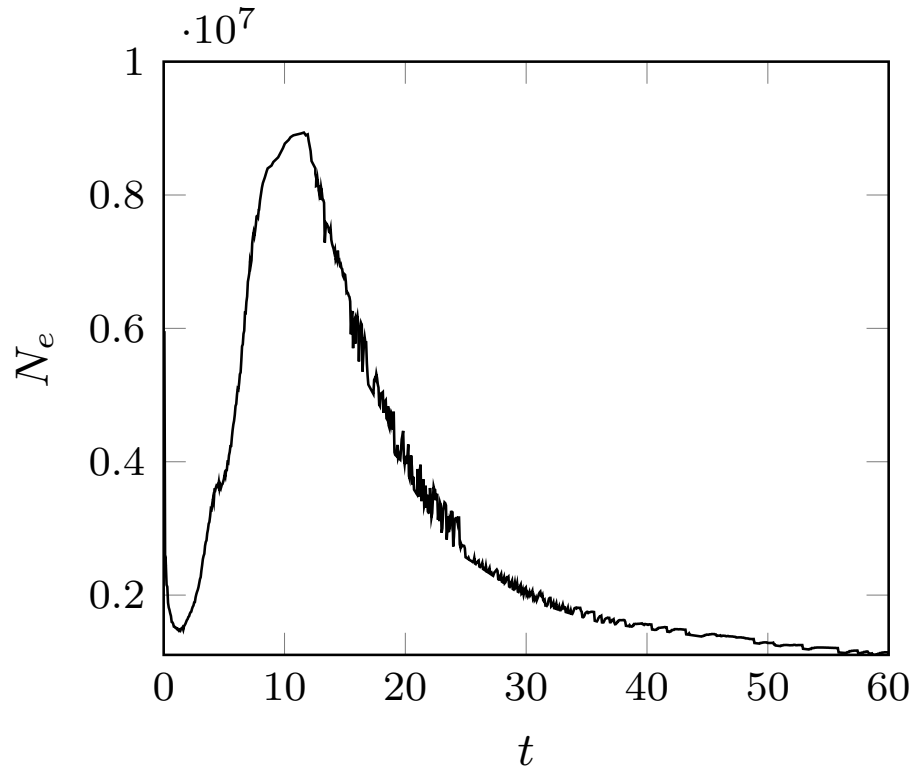


Fig. 6. Number of elements in the three-dimensional simulation as a function of time.

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page	
Abstract	Introduction
Conclusions	References
Tables	Figures
◀	▶
◀	▶
Back	Close
Full Screen / Esc	
Printer-friendly Version	
Interactive Discussion	



Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

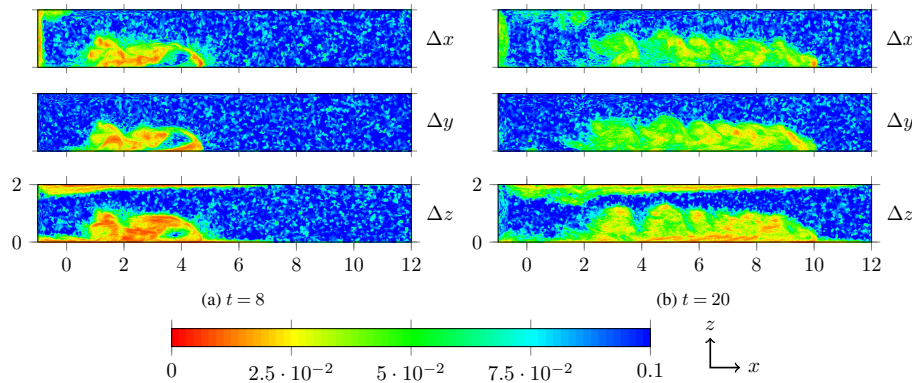


Fig. 7. Heatmap indicating the size of the elements in x , y and z across a plane at $y = 1.0$ and times $t = 8$ (left) and $t = 20$ (right).

Title Page

Abstract Introduction

Conclusions References

Tables Figures

⏪ ⏩

◀ ▶

Back Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



**Direct numerical
simulations of
particle-laden density
with finite-elements**

S. D. Parkinson et al.

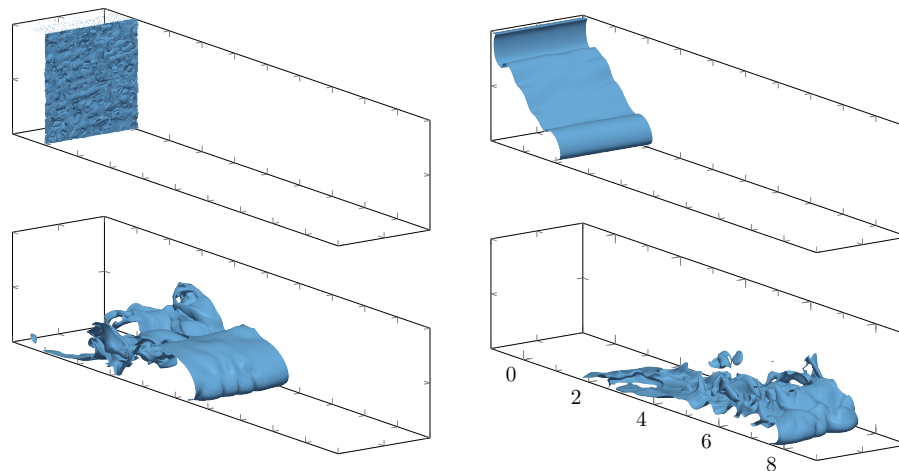


Fig. 8. Propagation of density interface over time. This figure shows a contour at a concentration 0.25 at times 0, 2, 8, and 14.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

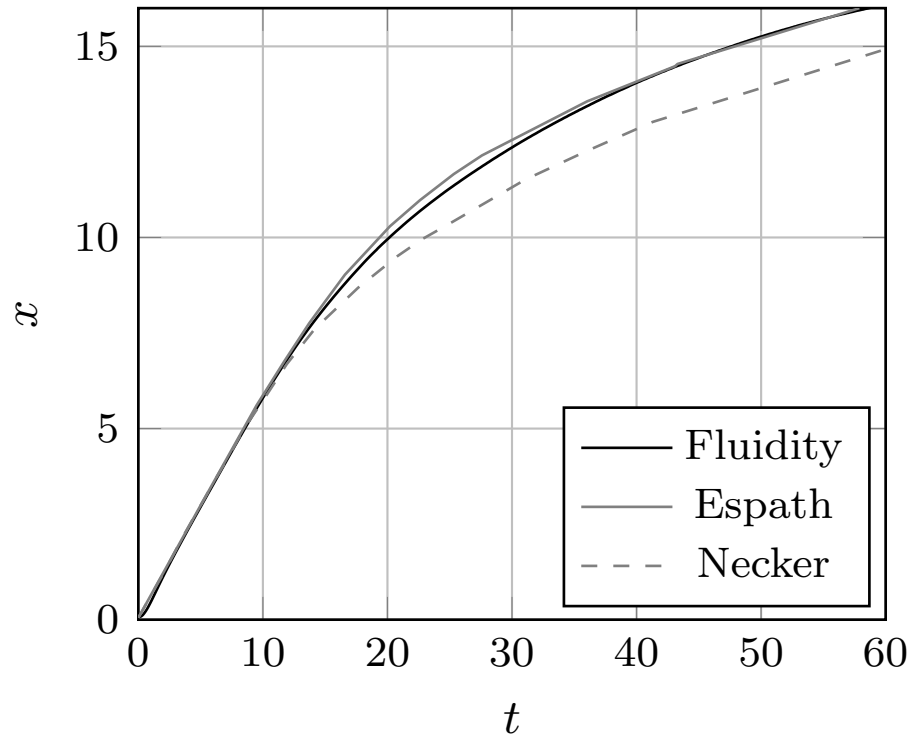


Fig. 9. Position of density current head against simulation time for the Fluidity simulation and the simulations of Necker et al. (2002) and Espath et al. (2014).

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

[Title Page](#)

[Abstract](#) [Introduction](#)

[Conclusions](#) [References](#)

[Tables](#) [Figures](#)

[⏪](#) [⏩](#)

[◀](#) [▶](#)

[Back](#) [Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)



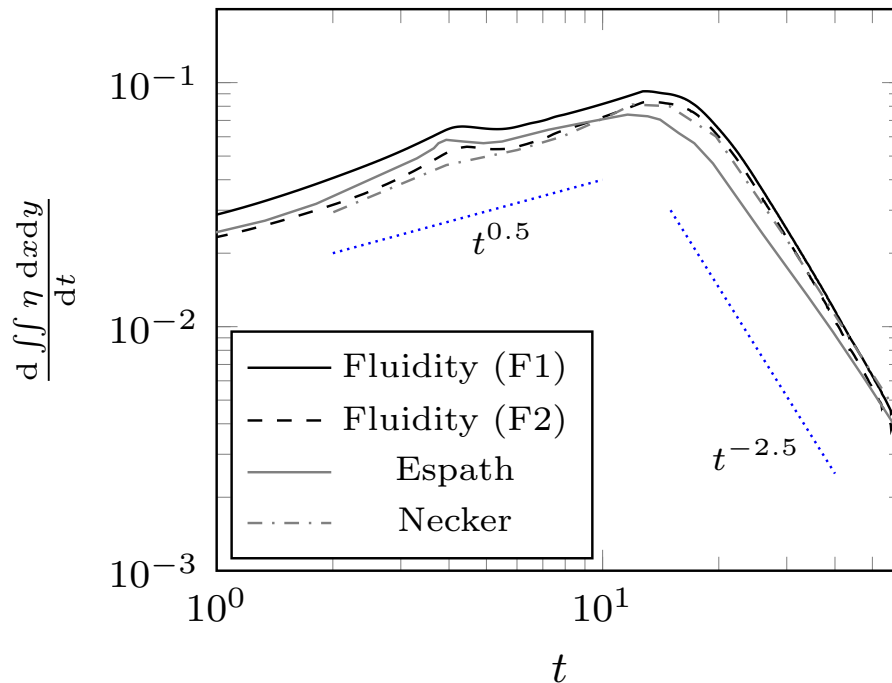


Fig. 10. Deposition rates for the three-dimensional simulation. Deposition rates from Fluidity (F1), Fluidity with a modified deposition rate where the erosion rate has been removed (F2), Espath et al. (2014), and Necker et al. (2002).

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

Title Page	
Abstract	Introduction
Conclusions	References
Tables	Figures
◀	▶
◀	▶
Back	Close
Full Screen / Esc	
Printer-friendly Version	
Interactive Discussion	



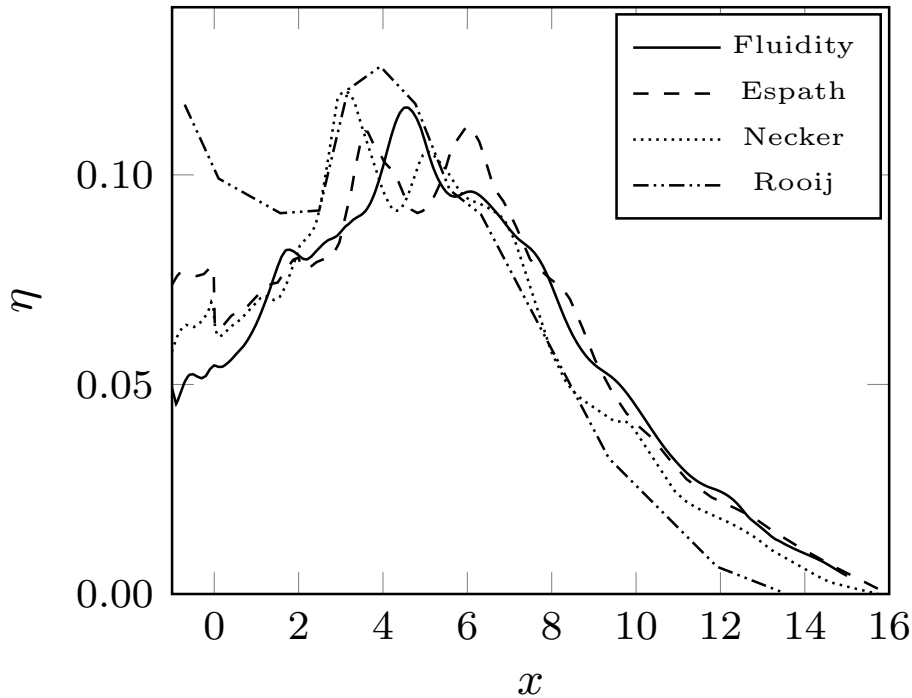


Fig. 11. Span-wise averaged deposit profile from the three dimensional simulation at $t = 60$. Comparisons are made against results from Necker et al. (2002); Espath et al. (2014) and De Rooij and Dalziel (2009).

Direct numerical simulations of particle-laden density with finite-elements

S. D. Parkinson et al.

[Title Page](#)

[Abstract](#) [Introduction](#)

[Conclusions](#) [References](#)

[Tables](#) [Figures](#)

[⏪](#) [⏩](#)

[◀](#) [▶](#)

[Back](#) [Close](#)

[Full Screen / Esc](#)

[Printer-friendly Version](#)

[Interactive Discussion](#)

