Particle methods
Part 2

Truncation error and consistency of particle methods

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What is accuracy and why do we care?

We need **convergence** **:**

$$\lim_{\substack{N\to\infty\\ \Delta t\to 0}}\begin{pmatrix}\text{numerical}\\ \text{solution}\end{pmatrix}=\begin{pmatrix}\text{exact solution}\\ \text{to PDE}\end{pmatrix}$$

The Lax Equivalence Theorem (crude version):

consistency + stability $\Rightarrow$ **convergence**

The Lax-Wendroff Theorem:

convergence + conservation $\Rightarrow$ convergence to the **correct (weak) solution!**

Hirsch (1990), Leveque (2002)

What is accuracy and why do we care?

The Lax-Wendroff Theorem:

convergence + conservation $\Rightarrow$ **weak solution to PDEs**

Without conservation, we might convervge, but maybe not to a real solution.

- shocks
- astrophysics (Monaghan, 2005)

Conservation and non-uniform h

Errors due to $h = h(x,t)$ studied by Hernquist (1993) – important in astrophsyics – errors ~10%

$$h = h(x,t) \qquad \Rightarrow \qquad \nabla W(\mathbf{x},h) = \nabla W(\mathbf{x},h)\big|_h + \frac{\partial W(\mathbf{x},h)}{\partial h}\nabla h$$

Additional terms can be derived – 10% CPU time cost.

Nelson and Papaloizou (1994)

"It seems one cannot have everything."

Monaghan (1992)

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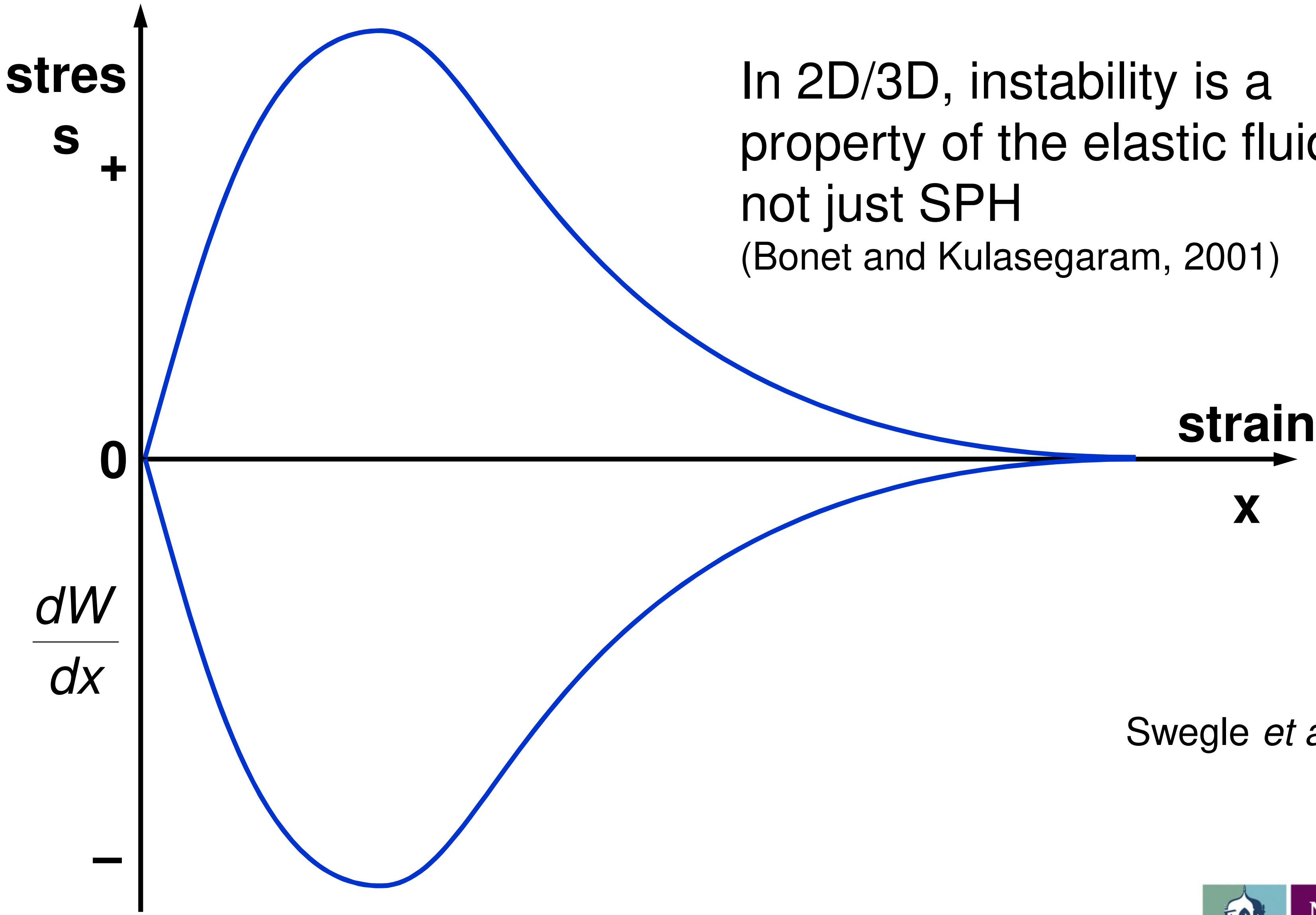
Tensile instability



In 2D/3D, instability is a property of the elastic fluid – not just SPH
(Bonet and Kulasegaram, 2001)

Swegle *et al*. (1995)

Remedies for tensile instability

Repulsive forces (Monaghan, 2000)

- maintain particle distribution
- non-physical momentum source

Total Lagrangian (Rabczuk et al., 2004)

- kernel is a function of material coordinates
- particle retains a constant material coordinate **X** and constant kernel values in **X** space
- suitable for very large deformation (fluids)?

Non-collocational (Dyka and Ingel, 1995)

- stress and velocity stored at different points

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Definitions

Consistency

(1) A **consistent** discrete approximation to a PDE exactly reproduces the PDE as $\Delta x \rightarrow 0$

Order of consistency

(2) A n^{th}-order consistent discrete approximation exactly reproduces n^{th}-order polynomials, always

=completeness, C^n

Consistency: statement of the problem

What is the error in the approximation

$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} \cong -\sum_b A(x_b)\frac{\partial W(x_b - x_a)}{\partial x_b}\Delta x_b \qquad \text{(1D)}$$

?

$$\left.\nabla A\right|_{\mathbf{x}=\mathbf{x}_a} \cong -\sum_b A(\mathbf{x}_b)\nabla_b W_a V_b \qquad \text{(2D/3D)}$$

Methods

Analysis

Taylor series expansions → truncation error in 1D

Numerical Experiments

Evaluation of an analytical test function

for:

- uniform and non-uniform particle distribution
- 1D and 3D
- standard SPH and consistency-corrected kernels

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The SPH evaluation of a gradient

Eulerian

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \frac{1}{\rho}\nabla p = 0$$

Lagrangian

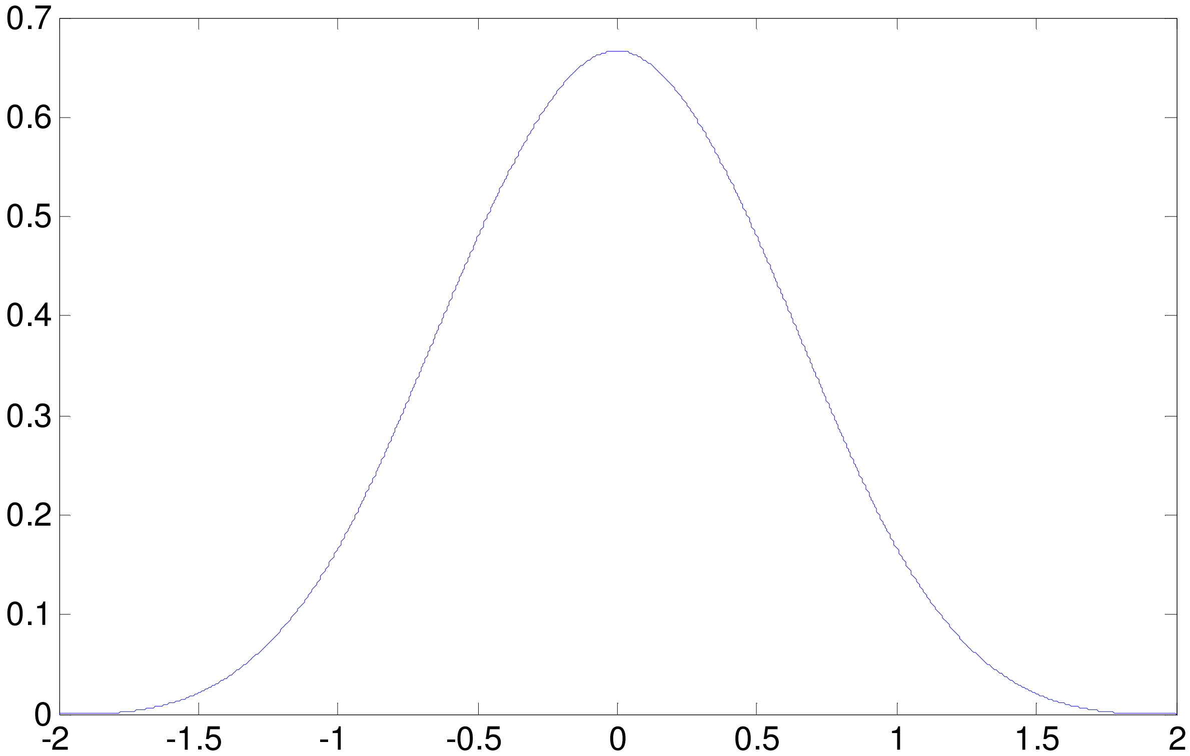
$$\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho}\nabla p = 0$$

$$\frac{\partial A(x_a)}{\partial x} \cong -\int_{x_a-2h}^{x_a+2h} A(x)\frac{\partial W(x-x_a)}{\partial x}dx \cong -\sum_b A(x_b)\frac{\partial W(x_b-x_a)}{\partial x_b}\Delta x_b$$

smoothing **discretisation**

The dimensionless kernel

$$\hat{W}(s) = hW(x - x_a)$$



$$s = \frac{x - x_a}{h}$$

Smoothing error

$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} \cong -\int_{x_a-2h}^{x_a+2h} A\frac{\partial W}{\partial x}dx$$

Expand $A(x)$ as a Taylor series and integrate by parts:

$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} = -\int_{x_a-2h}^{x_a+2h} A\frac{dW}{dx}dx + A'_a\left(1-\int_{x_a-2h}^{x_i+2h} Wdx\right) + \frac{1}{6}\left.\frac{\partial^3 A}{\partial x^3}\right|_a \int_{x_a-2h}^{x_a+2h}\left(x-x_a\right)^3\frac{\partial W}{\partial x}dx + \ldots$$

in dimensionless form:

$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} = -\int_{x_a-2h}^{x_a+2h} A\frac{\partial W}{\partial x}dx + A'_a\left(1-\int \hat{W}ds\right) + \frac{h}{2}A''_a\int s^2\hat{W}'ds + \frac{h^2}{6}A'''_a\int s^3\hat{W}'ds + \ldots$$

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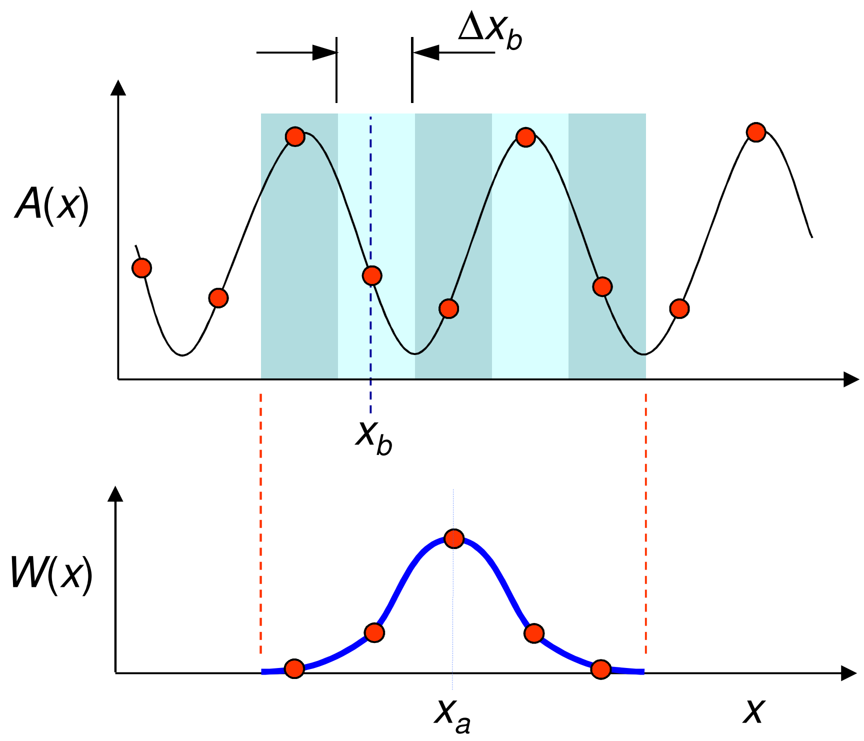
Discretisation error – special case

- Uniform particle spacing
- $\Delta x/h = 4/n$
- smooth kernel and data



general discretised form:

$$\int_{x_1-\Delta x/2}^{x_n+\Delta x/2} f(x)dx \cong \Delta x \sum_{b=1}^{n} f(x_b)$$

The 2nd Euler-MacLaurin Formula:

$$\int_{x_1-\Delta x/2}^{x_n+\Delta x/2} f(x)dx = \Delta x \sum_{b=1}^{n} f(x_b) - \sum_{k=1}^{\infty} \frac{B_{2k}\Delta x^{2k}}{(2k)!}\left(1-2^{-2k+1}\right)\left(f_{(n+1/2)}^{(2k-1)} - f_{(1/2)}^{(2k-1)}\right)$$

Ralston (1965), Quinlan *et al*. (2005)

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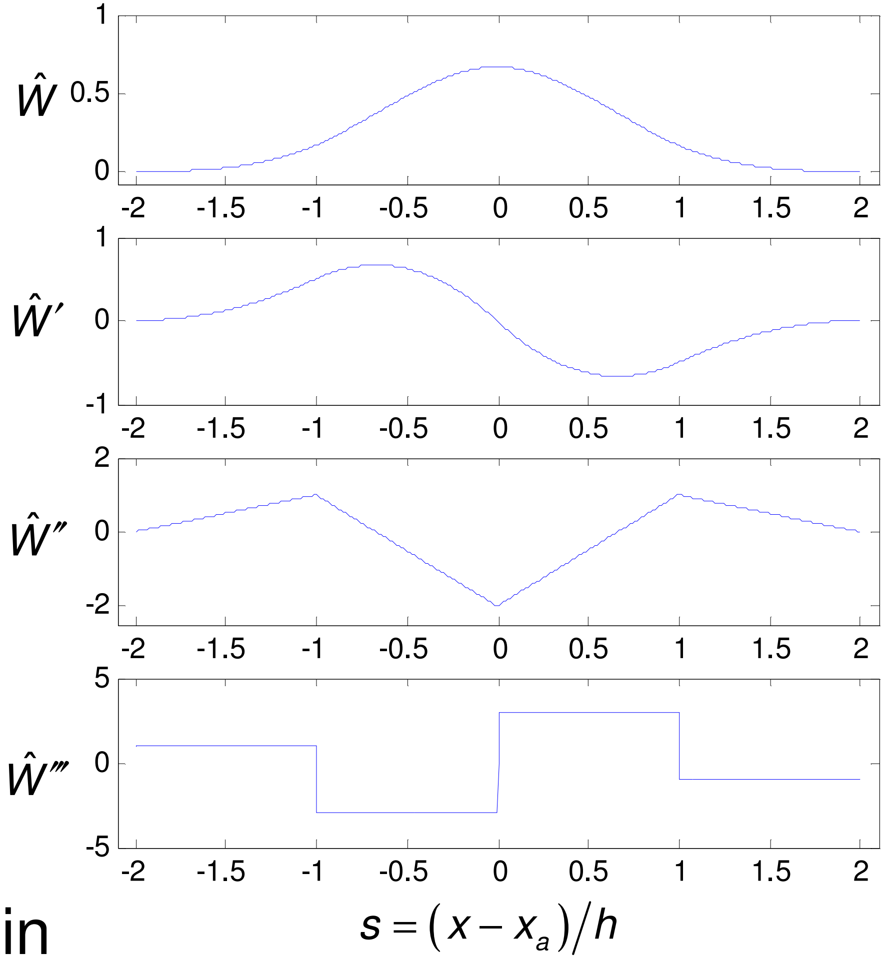
Kernel boundary smoothness

Boundary smoothness of the kernel is the highest integer β for which the β^{th} derivative and all lower derivatives are zero at the boundaries of the compact support.

cubic B-spline kernel



cubic B-spline: β=2

Gaussian: $\beta \rightarrow \infty$ in infinite domain

polynomial: arbitrary β

Overall error – uniform particle spacing

SPH estimate

exact derivative

$$-\sum_b A_b W_b' \Delta x_b = \left.\frac{\partial A}{\partial x}\right|_{x=x_a}$$

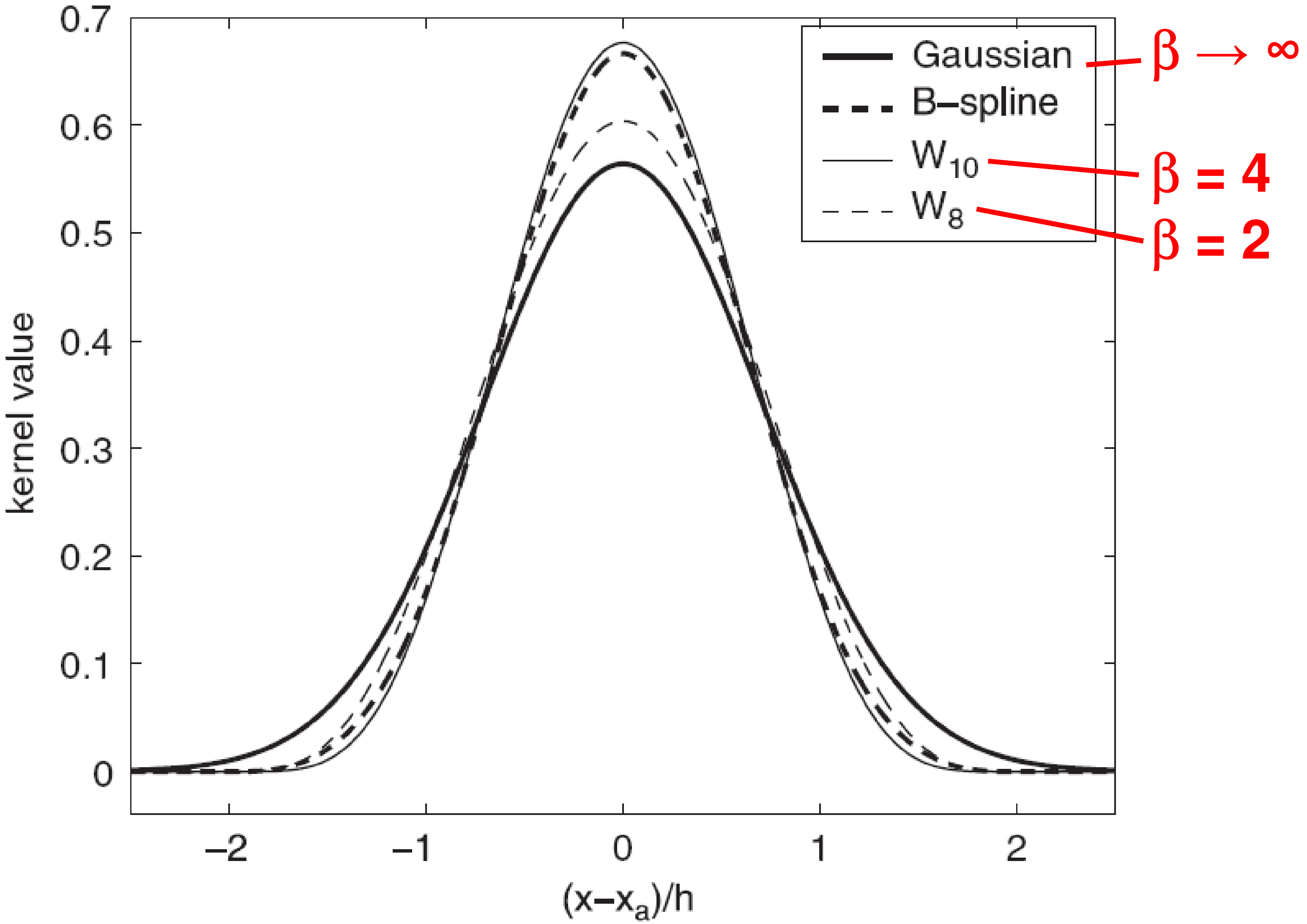
$$+\frac{h^2}{6} A_a''' \int s^3 \hat{W}' ds + \ldots$$

smoothing error

$$-\left(\frac{\Delta x}{h}\right)^{\beta+2} \frac{B_{\beta+2}}{(\beta+2)!}\left(1-2^{-\beta-1}\right)\left[A_a'\left(4\hat{W}_{s=2}^{(\beta+2)}+2(\beta+1)\hat{W}_{s=2}^{(\beta+1)}\right)+O\left(h^2\right)\right]-\ldots$$

discretisation error

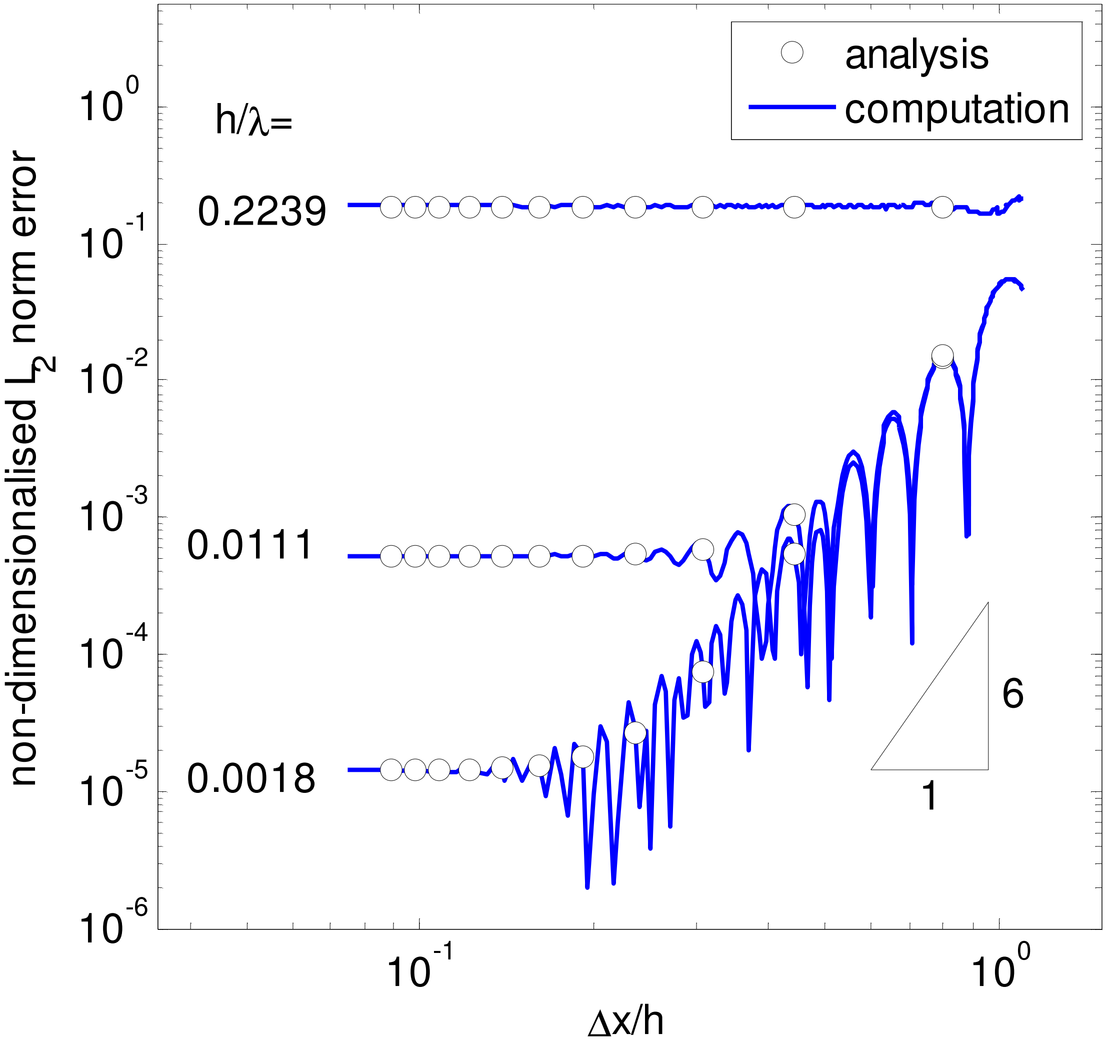
Kernels for testing



Results – uniform particle spacing, 1D

sinusoidal test function $A(x)$, wavelength λ

10^{th} order polynomial kernel, $\beta=4$



Results – uniform particle spacing, 1D

sinusoidal test function $A(x)$, wavelength λ

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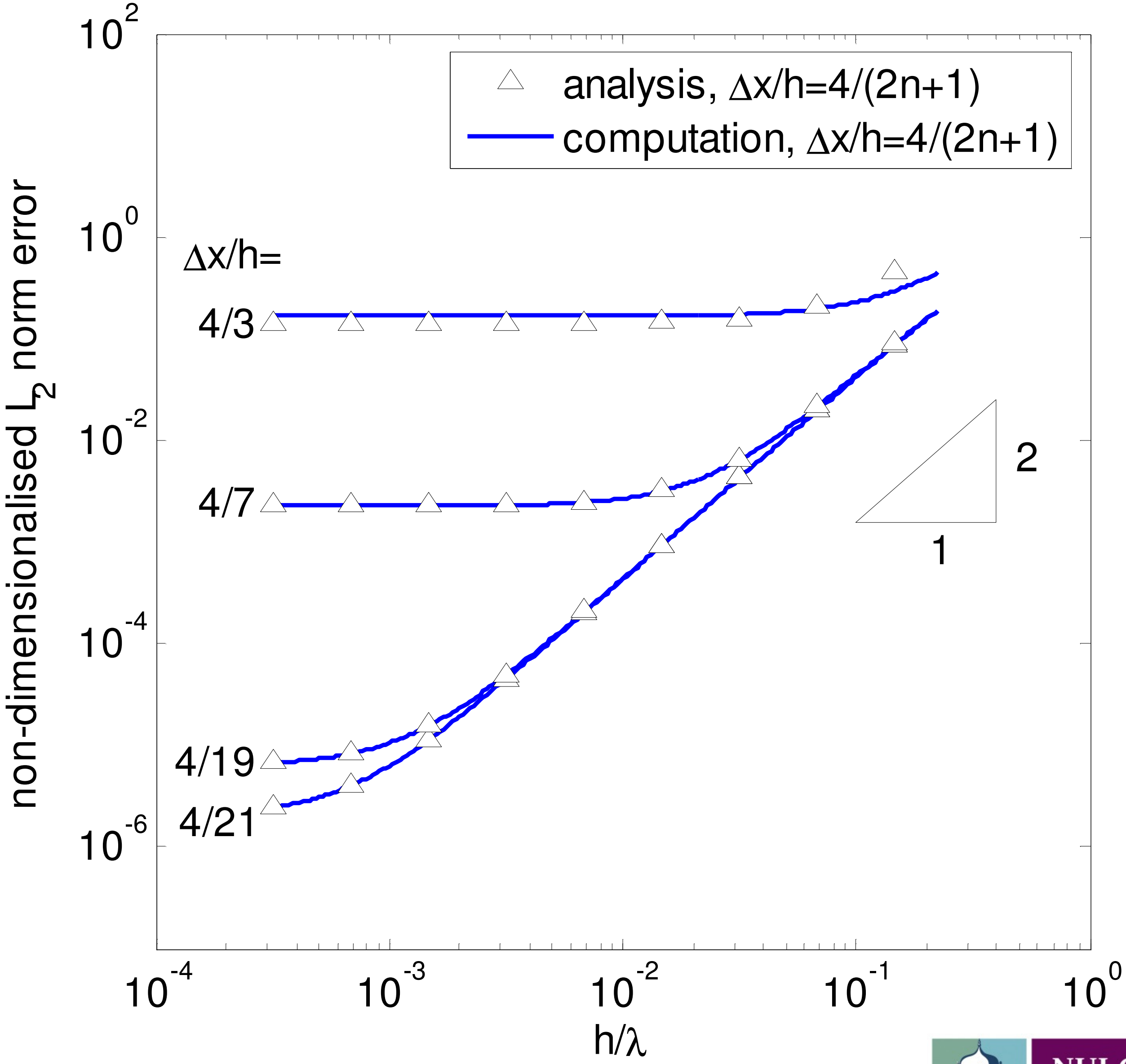

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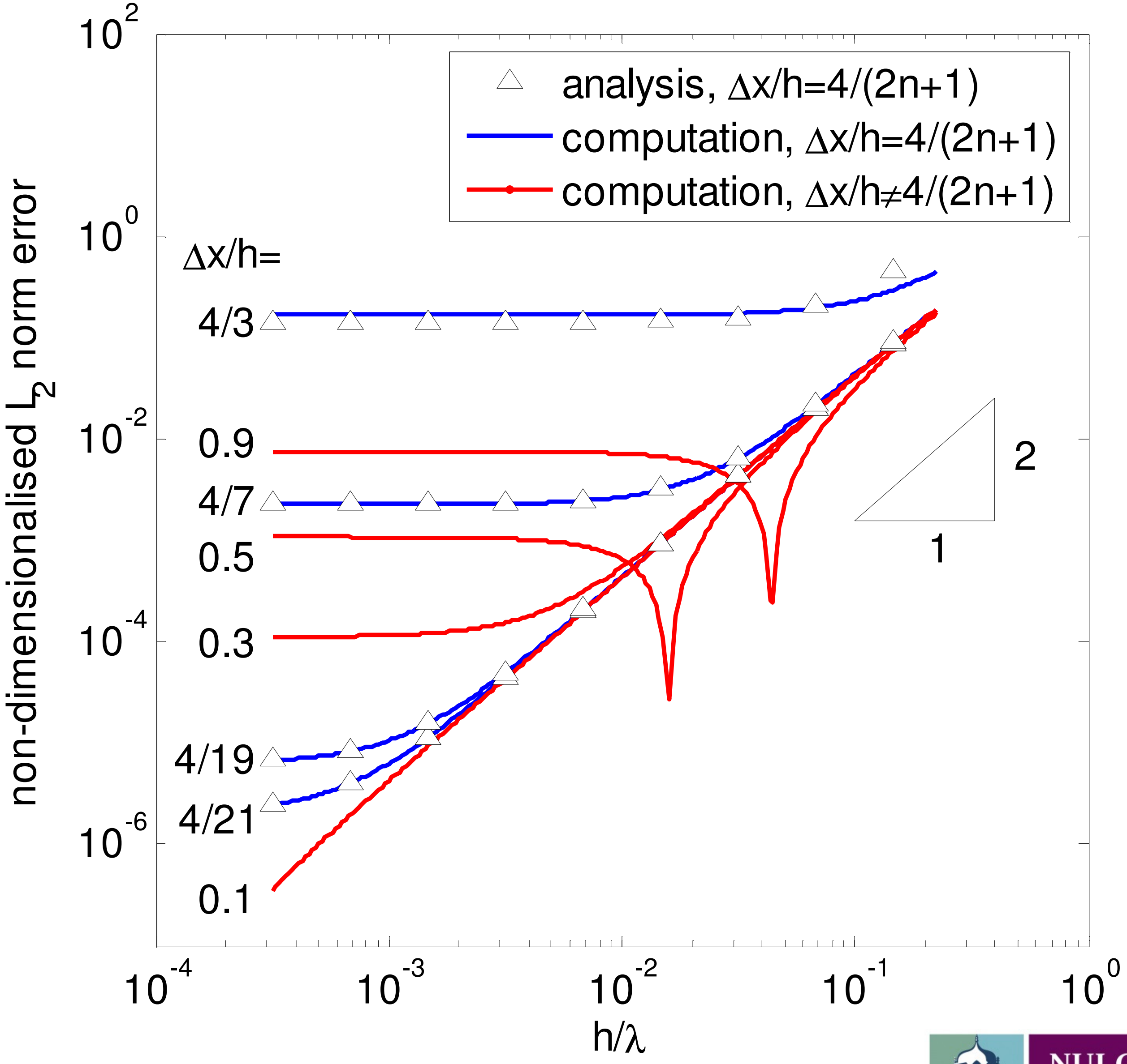
Results – uniform particle spacing, 1D

sinusoidal test function *A*(*x*), wavelength λ

10th order polynomial kernel, β=4



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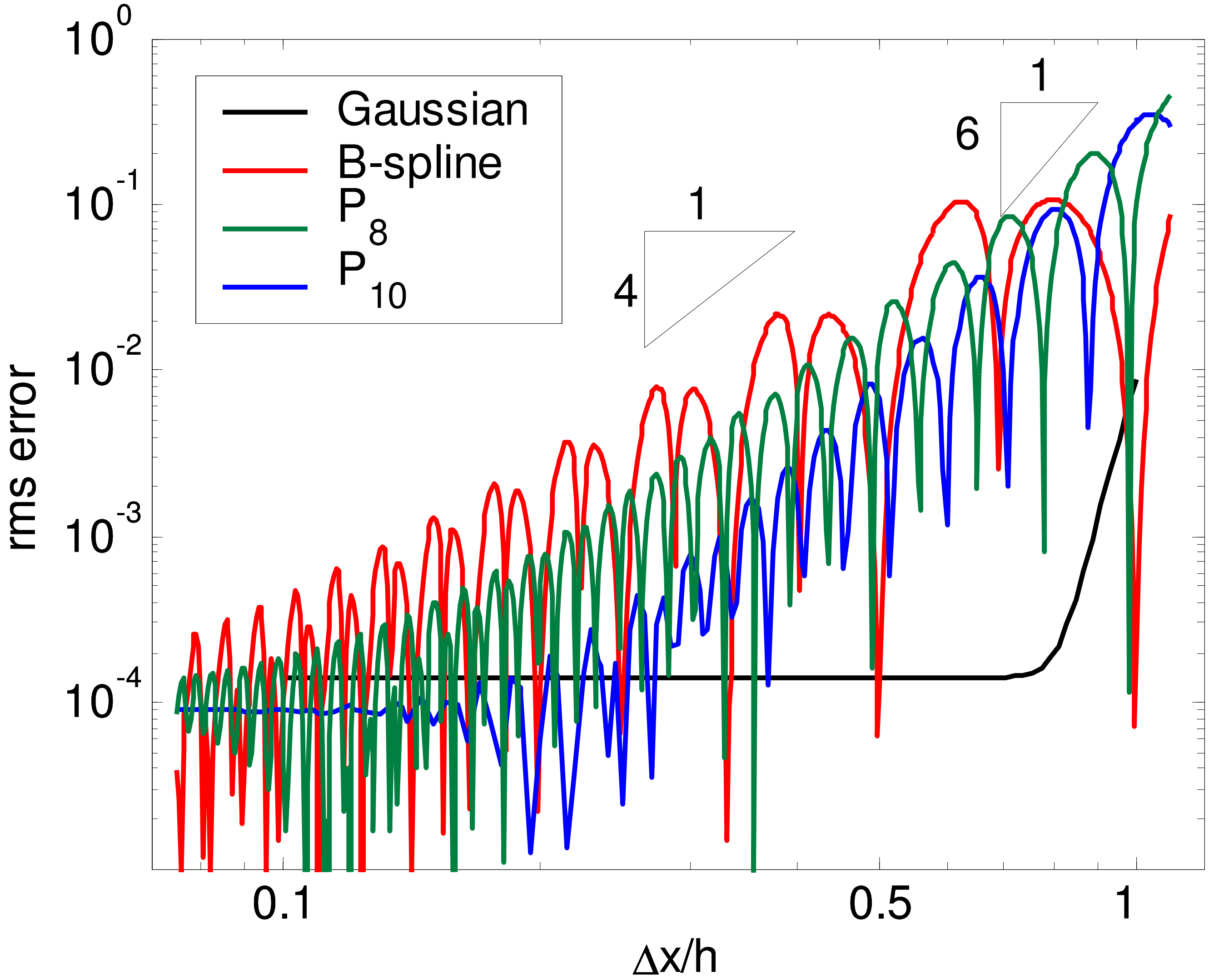
Kernel comparison

Sinusoidal test function, wavelength λ

empirical results

$h/\lambda = 0.0018$



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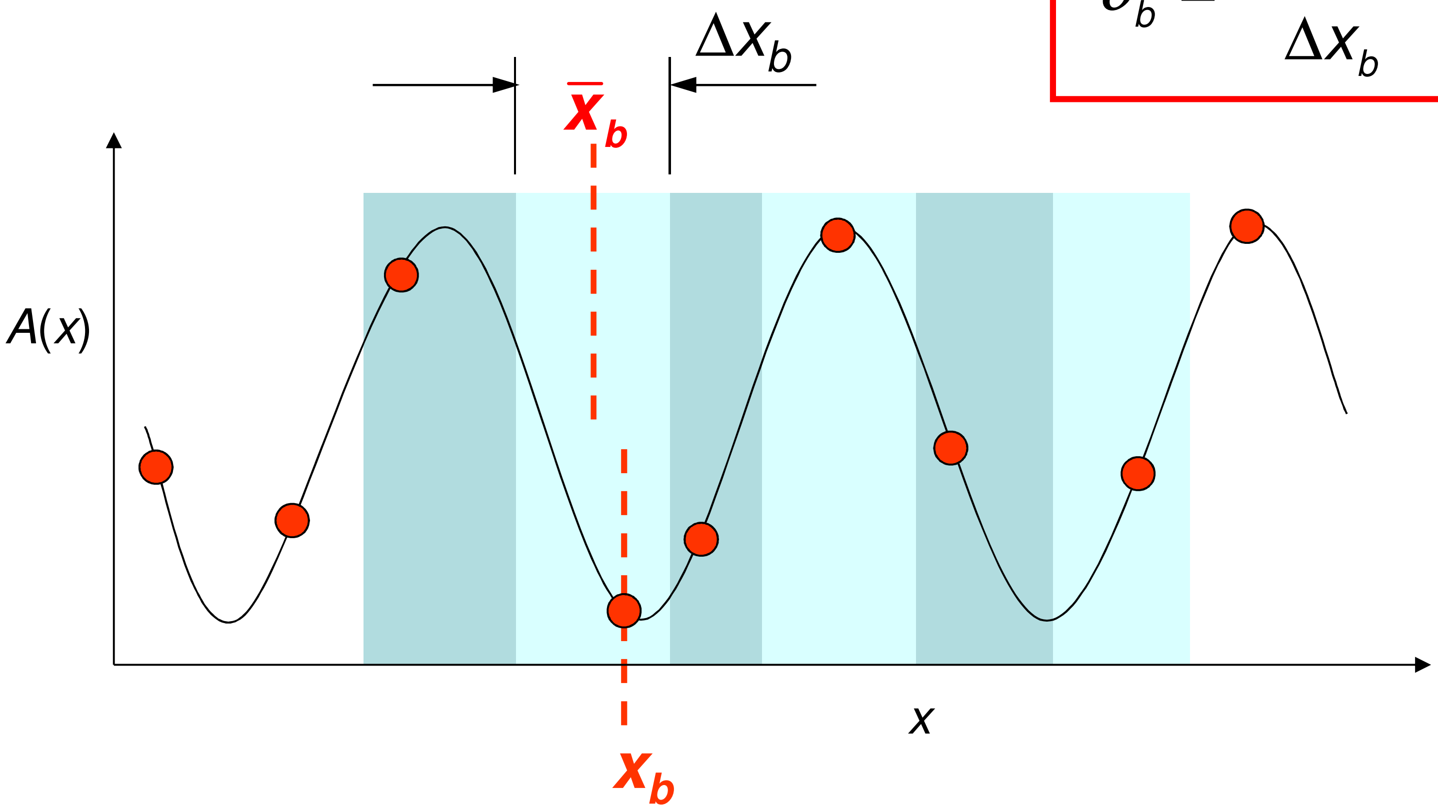
Non-uniform particle distribution

x_b is the location of particle b

$\overline{x}_b$ is the centroid of a region associated with particle b

$$\boxed{\delta_b = \frac{x_b - \overline{x}_b}{\Delta x_b}}$$



Non-uniform spacing

$$-\sum_b A_b W_b' \Delta x_b = \left.\frac{\partial A}{\partial x}\right|_{x=x_a}$$

$$- A_a'\left(\int \hat{W} ds - 1\right) + \frac{h^2}{6} A_a''' \int s^3 \hat{W}' ds + \dots$$

smoothing error

$$-\frac{1}{h}\left[A_a \delta O\left(\left(\frac{\Delta x}{h}\right)^3\right) + \frac{A_a}{2}\left(\delta^2+\frac{1}{12}\right)O\left(\left(\frac{\Delta x}{h}\right)^4\right)\right]$$

$$-\left[A_a'\delta O\left(\left(\frac{\Delta x}{h}\right)^3\right)\right]$$

$$-h\left[\frac{A_a''}{2}\delta O\left(\frac{\Delta x}{h}\right) + \frac{A_a''}{2} O\left(\left(\frac{\Delta x}{h}\right)^4\right)\right] - \dots$$

discretisation error

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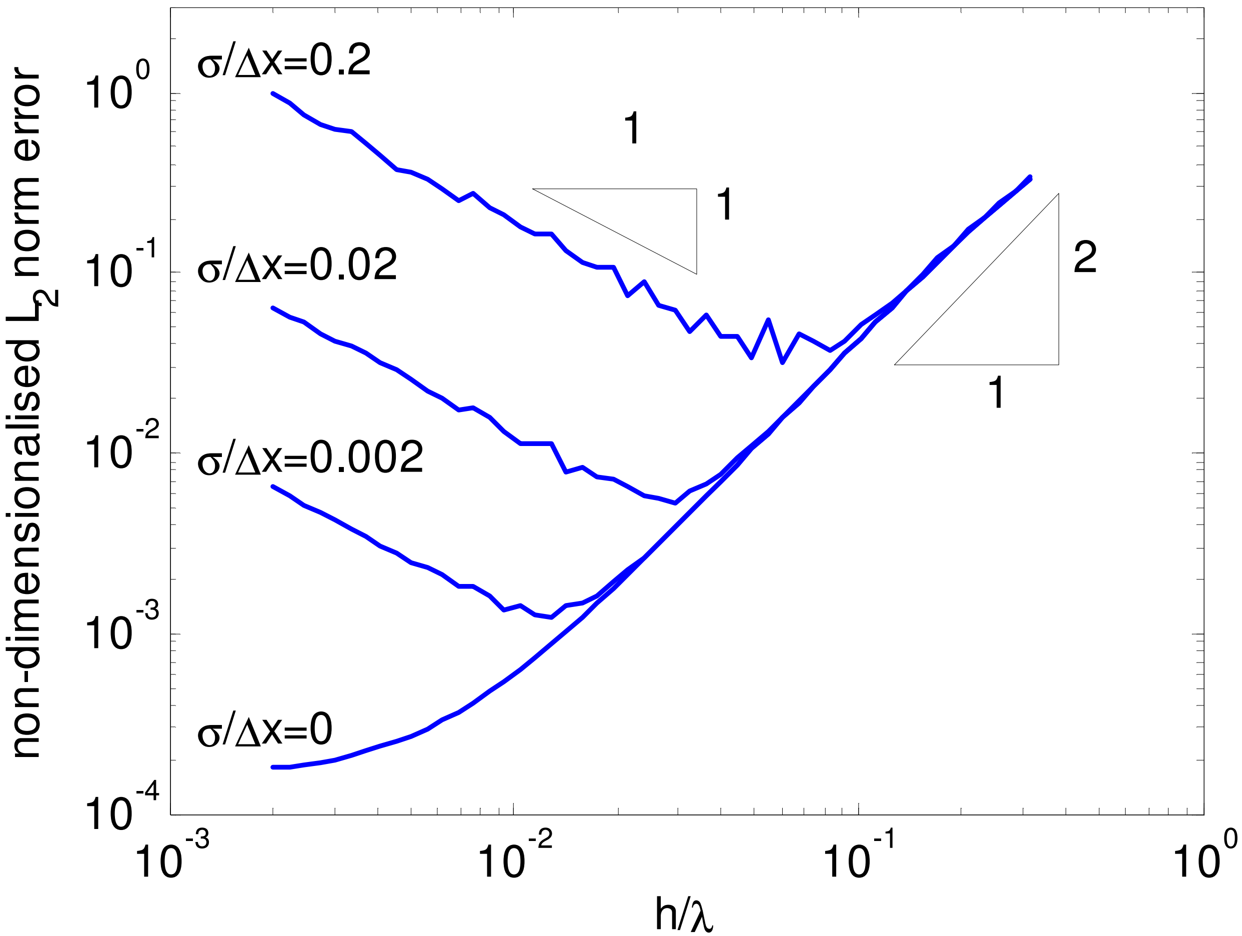
Non-uniform spacing – results

Normally distributed random perturbation of standard deviation σ imposed on uniform particle distribution.

sinusoidal test function, wavelength λ

10^{th} order polynomial kernel, β=4

$\Delta x/h = 0.364$



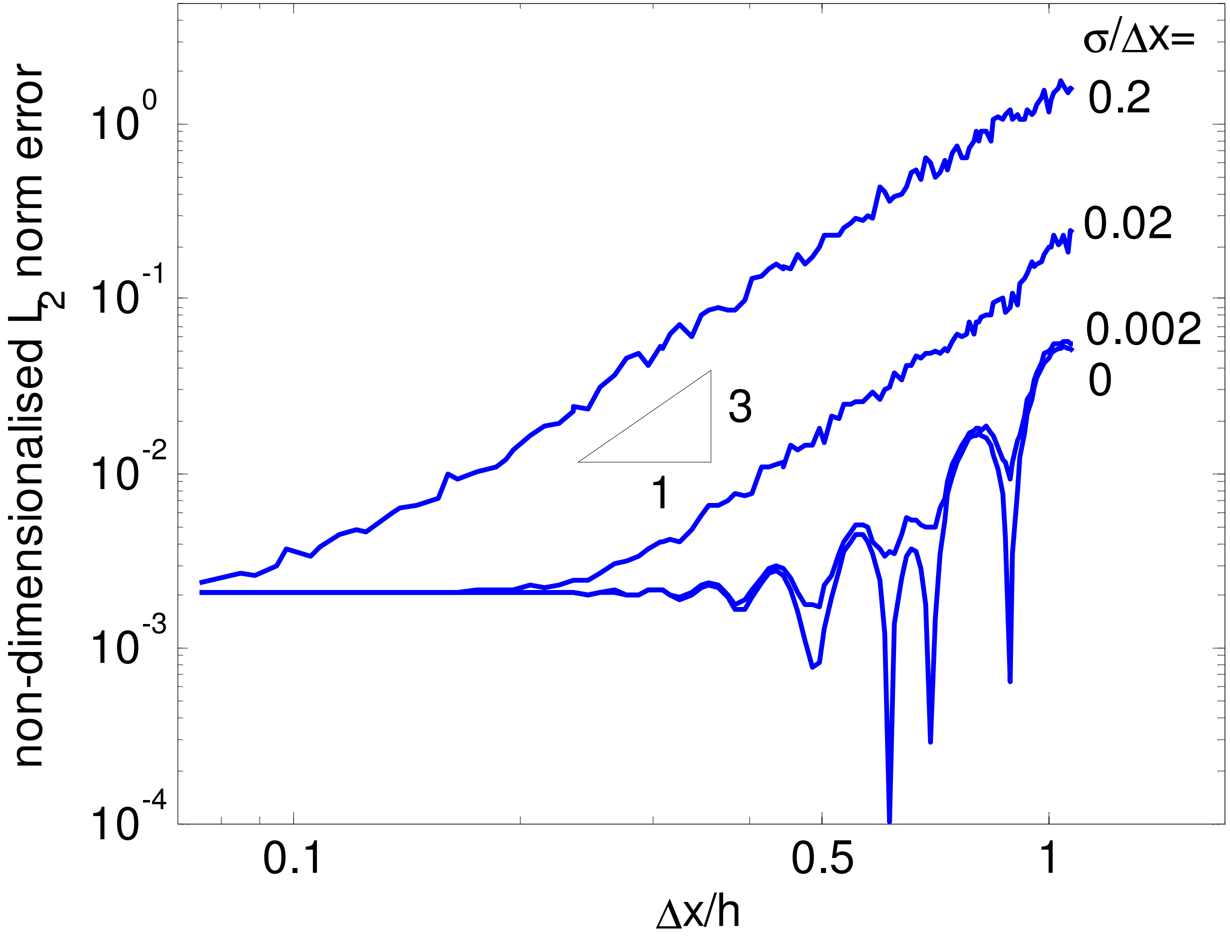
Non-uniform spacing – results

Normally distributed random perturbation of standard deviation σ imposed on uniform particle distribution.

sinusoidal test function, wavelength λ

10^{th} order polynomial kernel, β=4

$h/\lambda = 0.022$



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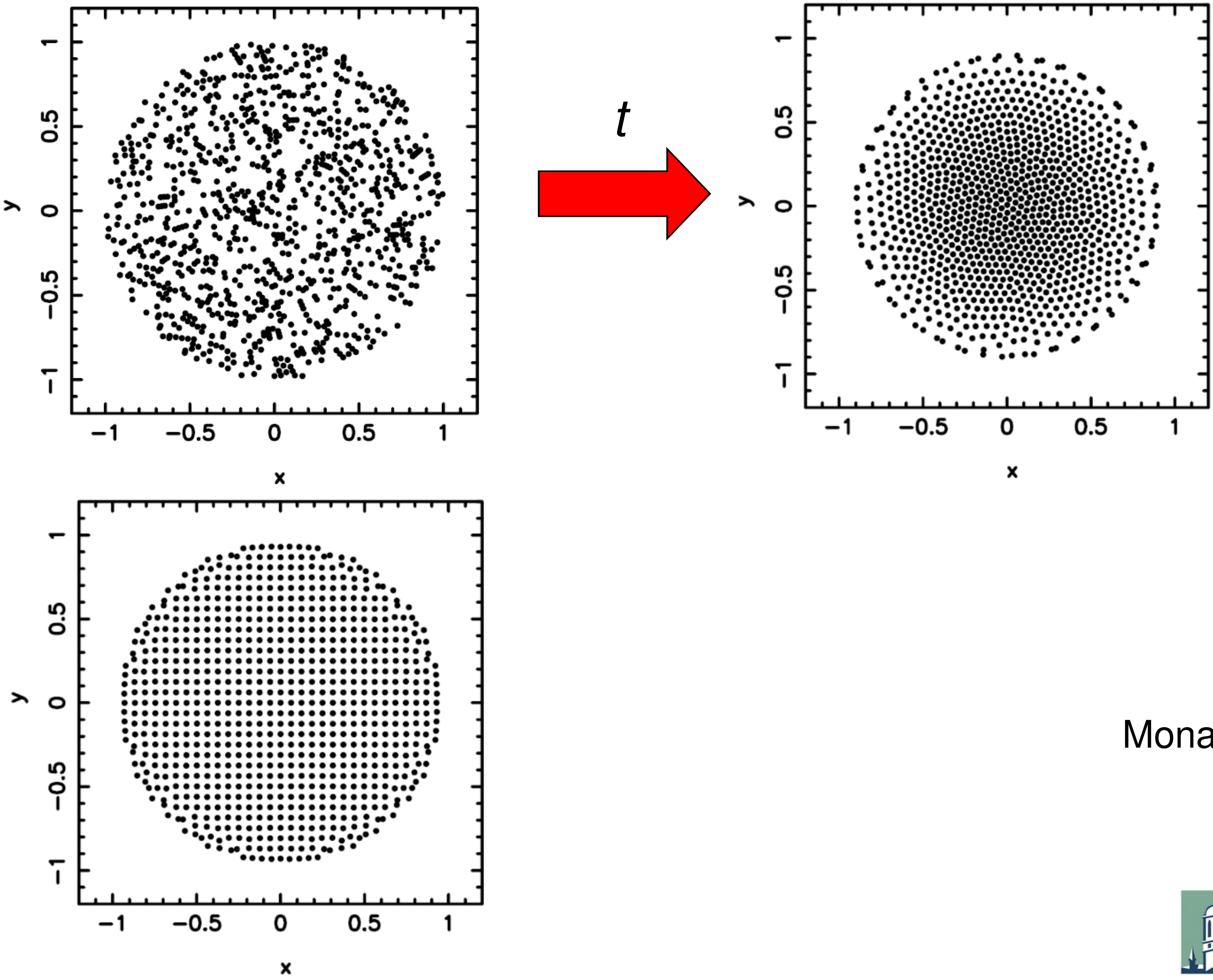
Is randomness a good model for measuring error?



Monaghan (2005)

Designing kernels for higher orders of consistency

Corrected SPH (CSPH) (Bonet and Lok, 1999; Vignjevic et al., 2000)

$$\tilde{W}(\mathbf{x}_b - \mathbf{x}) = \frac{W(\mathbf{x}_b - \mathbf{x})}{\sum_b W(\mathbf{x}_b - \mathbf{x}) V_b}$$

zero-order consistent kernel

$$\left(\sum_b \mathbf{x}_b^T \nabla \tilde{W}(\mathbf{x}_b - \mathbf{x}) V_b \right)^{-1} \nabla \tilde{W}$$

first-order consistent kernel gradient

Reproducing Kernel Particle Method (RKPM) (Liu et al., 1995)

$$\sum_b W(\mathbf{x}_b - \mathbf{x}) \mathbf{P}(\mathbf{x}_b) \mathbf{P}(\mathbf{x}_b - \mathbf{x})^T \mathbf{c}(\mathbf{x}) = \mathbf{P}(\mathbf{x})$$

$$\tilde{W}(\mathbf{x} - \mathbf{x}_a) = \mathbf{c}\mathbf{P}(\mathbf{x}) W(\mathbf{x} - \mathbf{x}_a)$$

first-order consistent kernel

Designing kernels for higher orders of consistency

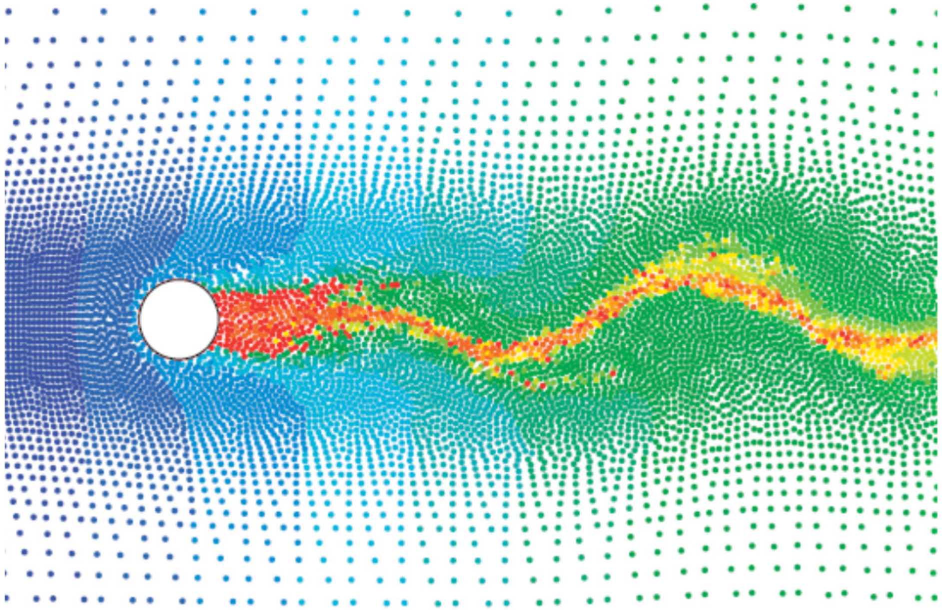
Pro

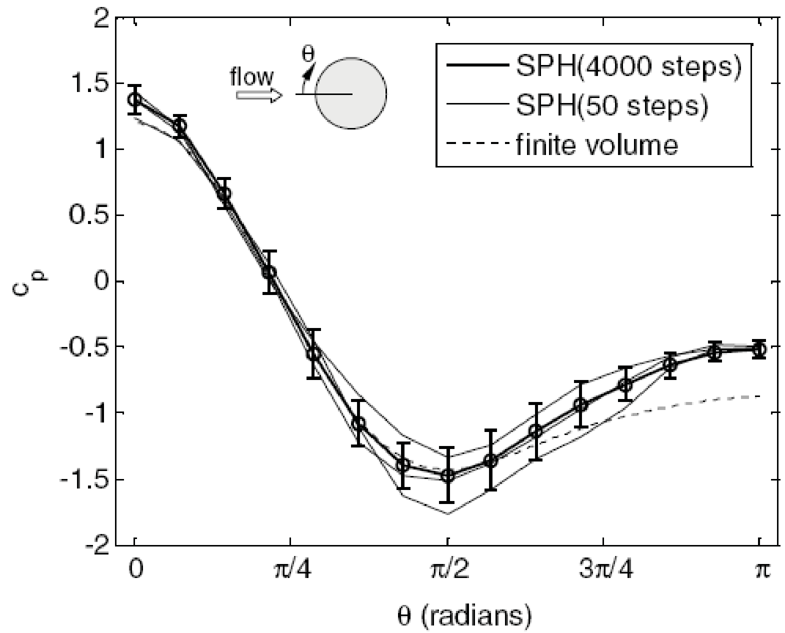
- Better approximations near non-uniform particle distributions
- Better approximations near boundaries
- Less prone to tensile instability? (Bonet and Kulasegaram, 2001)

Con

- Corrections must be computed per particle
- Computational effort
- Loss of SPH conservation properties

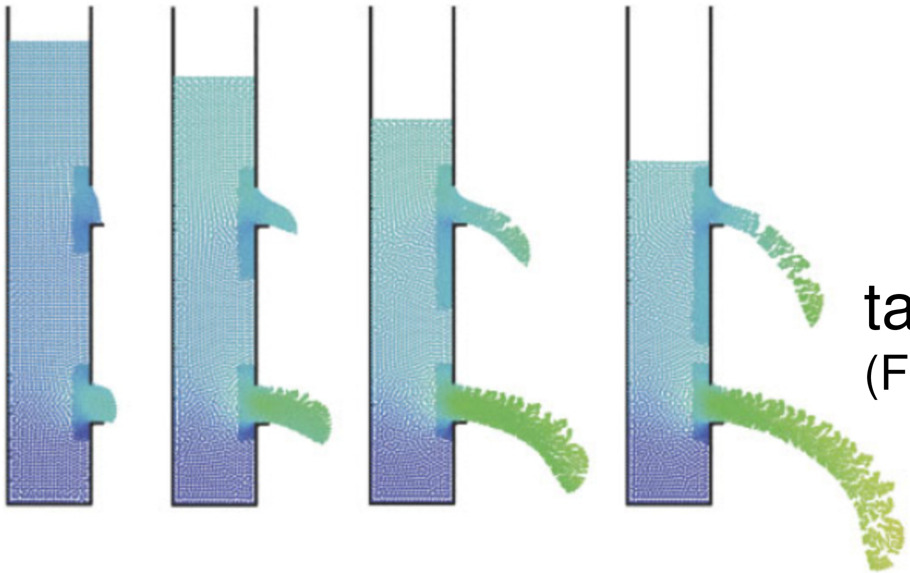
Consistency-corrected SPH results





cylinder at Re_d = 100

(Lastiwka *et al*., 2008)



tank empyting

(Feldman and Bonet, 2007)

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Truncation error with consistency-corrected kernels

A n^{th}-order consistent kernel ensures exact calculation of gradients of polynomials up to order n.

A general expression for error:

$$\varepsilon = \varepsilon_d + \varepsilon_s = \alpha_0\left(h,\frac{\Delta x}{h},\delta\right)A_a + \alpha_1\left(h,\frac{\Delta x}{h},\delta\right)A'_a + \alpha_2\left(h,\frac{\Delta x}{h},\delta\right)A''_a + \dots$$

For a first-order consistent kernel, by definition:

$$\alpha_0 = \alpha_1 = 0$$

Truncation error for first-order consistent kernel

$$-\sum_b A_b W_b' \Delta x_b = \left.\frac{\partial A}{\partial x}\right|_{x=x_a}$$

$$\left.\begin{array}{l} - A_a'\left(\int \hat{W} ds - 1\right) + \frac{h}{2} A_a'' \int s^2 \hat{W}' ds + \frac{h^2}{6} A_a''' \int s^3 \hat{W}' ds + \ldots \end{array}\right\}$$

smoothing error

$$-\frac{1}{h}\left[A_a \delta O\left(\left(\frac{\Delta x}{h}\right)^3\right) + \frac{A_a}{2}\left(\delta^2 + \frac{1}{12}\right) O\left(\left(\frac{\Delta x}{h}\right)^4\right)\right]$$

$$-\left[A_a' \delta O\left(\left(\frac{\Delta x}{h}\right)^3\right)\right]$$

$$-h\left[\frac{A_a''}{2} \delta O\left(\frac{\Delta x}{h}\right) + \frac{A_a''}{2} O\left(\left(\frac{\Delta x}{h}\right)^4\right)\right] - \ldots$$

discretisation error

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First-order consistent kernel

$$-\sum_b A_b W_b' \Delta x_b = \left.\frac{\partial A}{\partial x}\right|_{x=x_a}$$

$$\left.\begin{array}{l} + \dfrac{h}{2} A_a'' \int s^2 \hat{W}' ds + \dfrac{h^2}{6} A_a''' \int s^3 \hat{W}' ds + \ldots \end{array}\right\}$$ **smoothing error**

$$\left.\begin{array}{l} - h\left[\dfrac{A_a''}{2} \delta O\left(\dfrac{\Delta x}{h}\right) + \dfrac{A_a''}{2} O\left(\left(\dfrac{\Delta x}{h}\right)^4\right)\right] - \ldots \end{array}\right\}$$ **discretisation error**

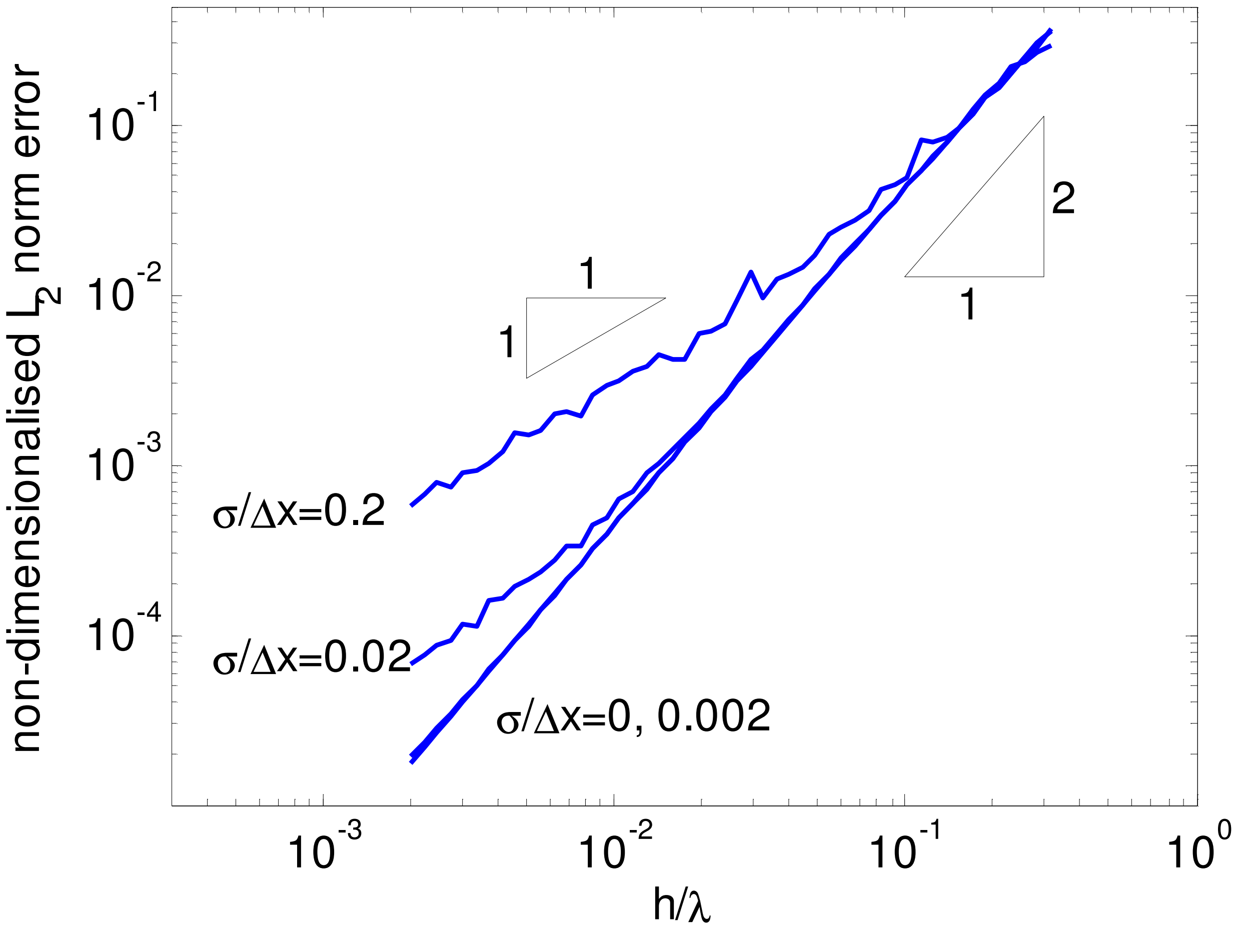
First-order consistent kernel – numerical results

First-order convergence observed in discretisation-limited error

sinusoidal test function, wavelength λ

10th order polynomial kernel, β=4

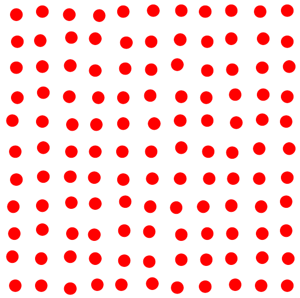
$\Delta x/h = 0.7$

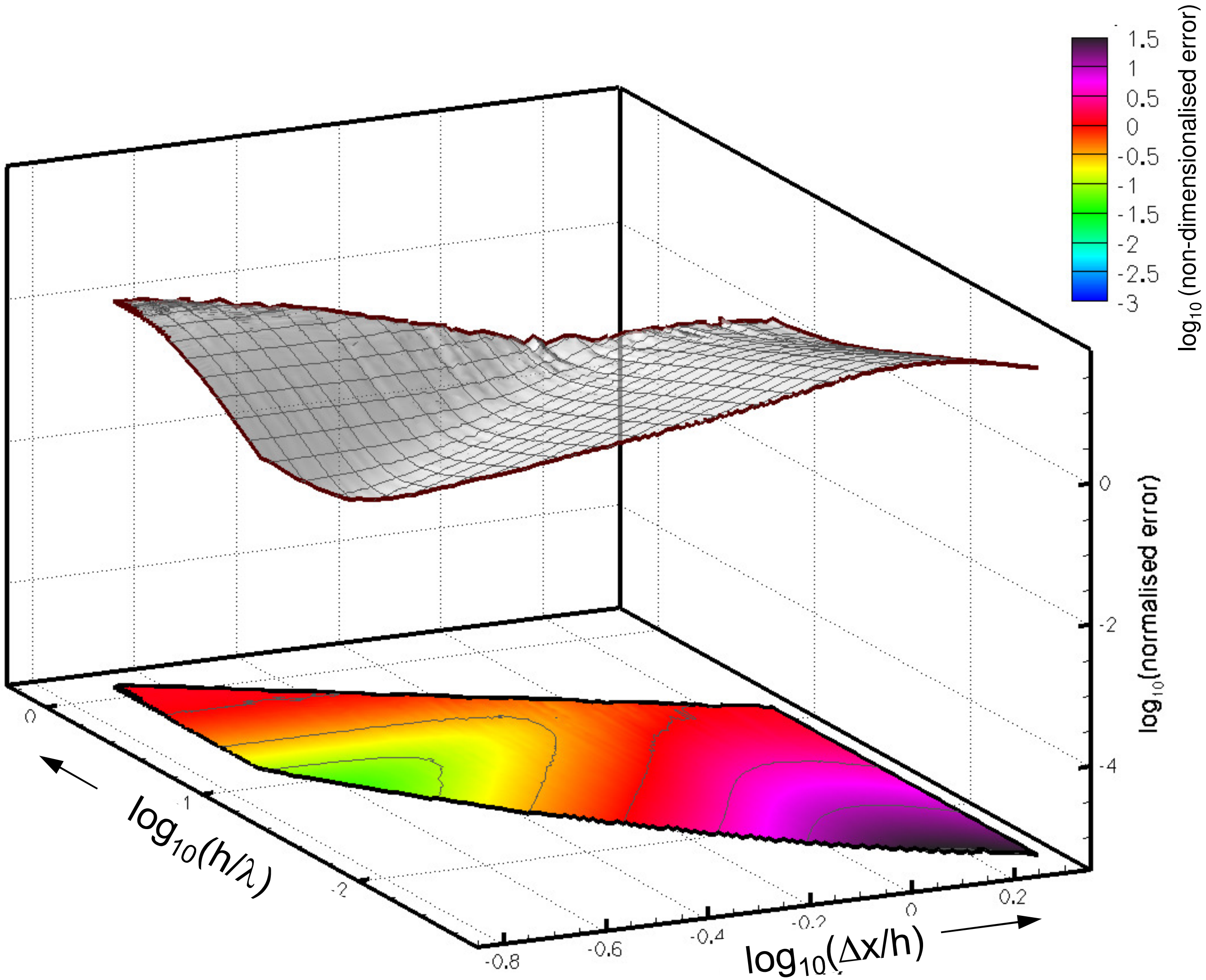


3D standard SPH

$\sigma/\Delta x = 0.2$

(high disorder)

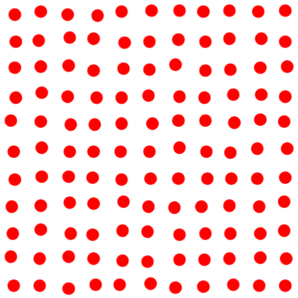


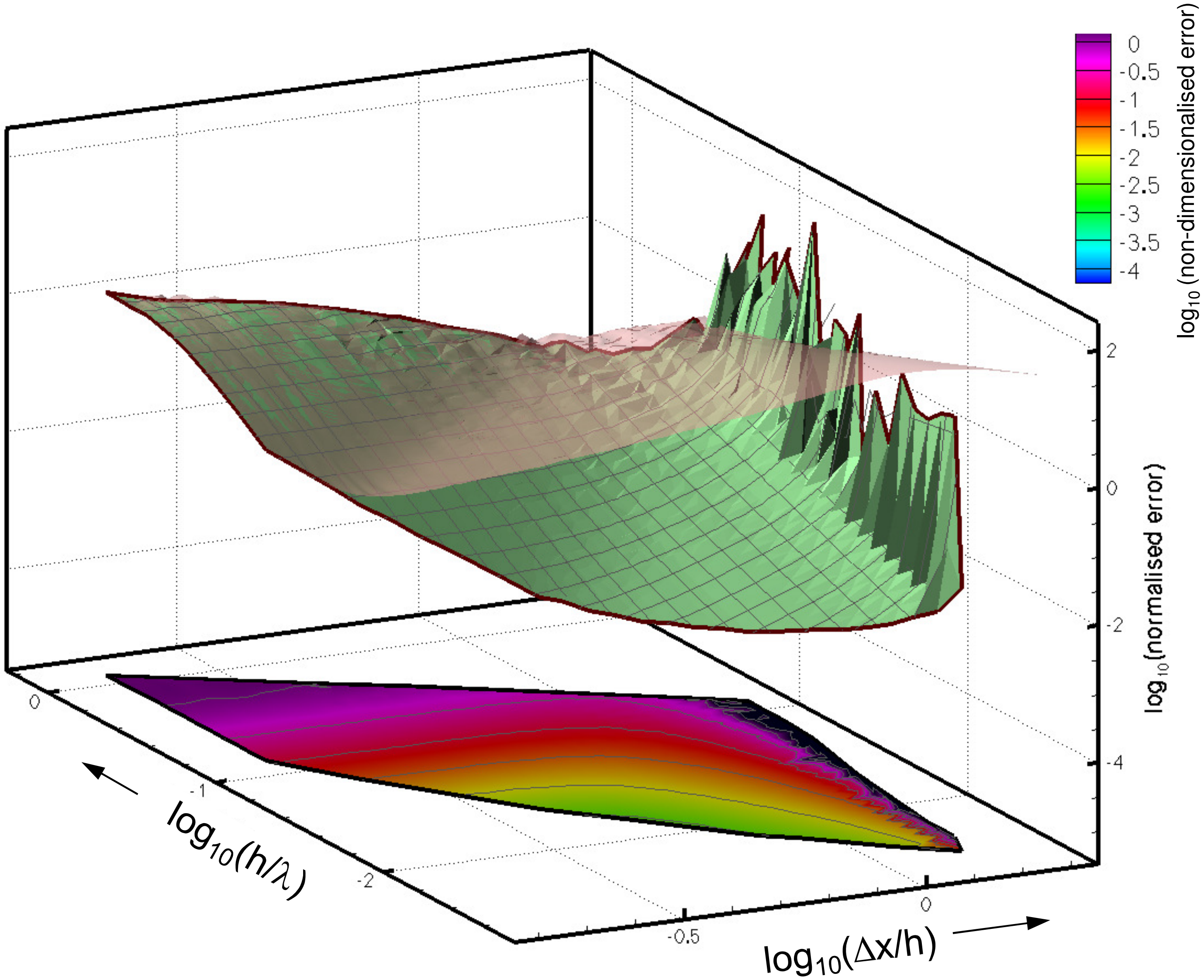


3D standard and corrected SPH

$\sigma/\Delta x = 0.2$

(high disorder)

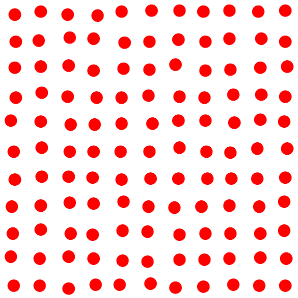


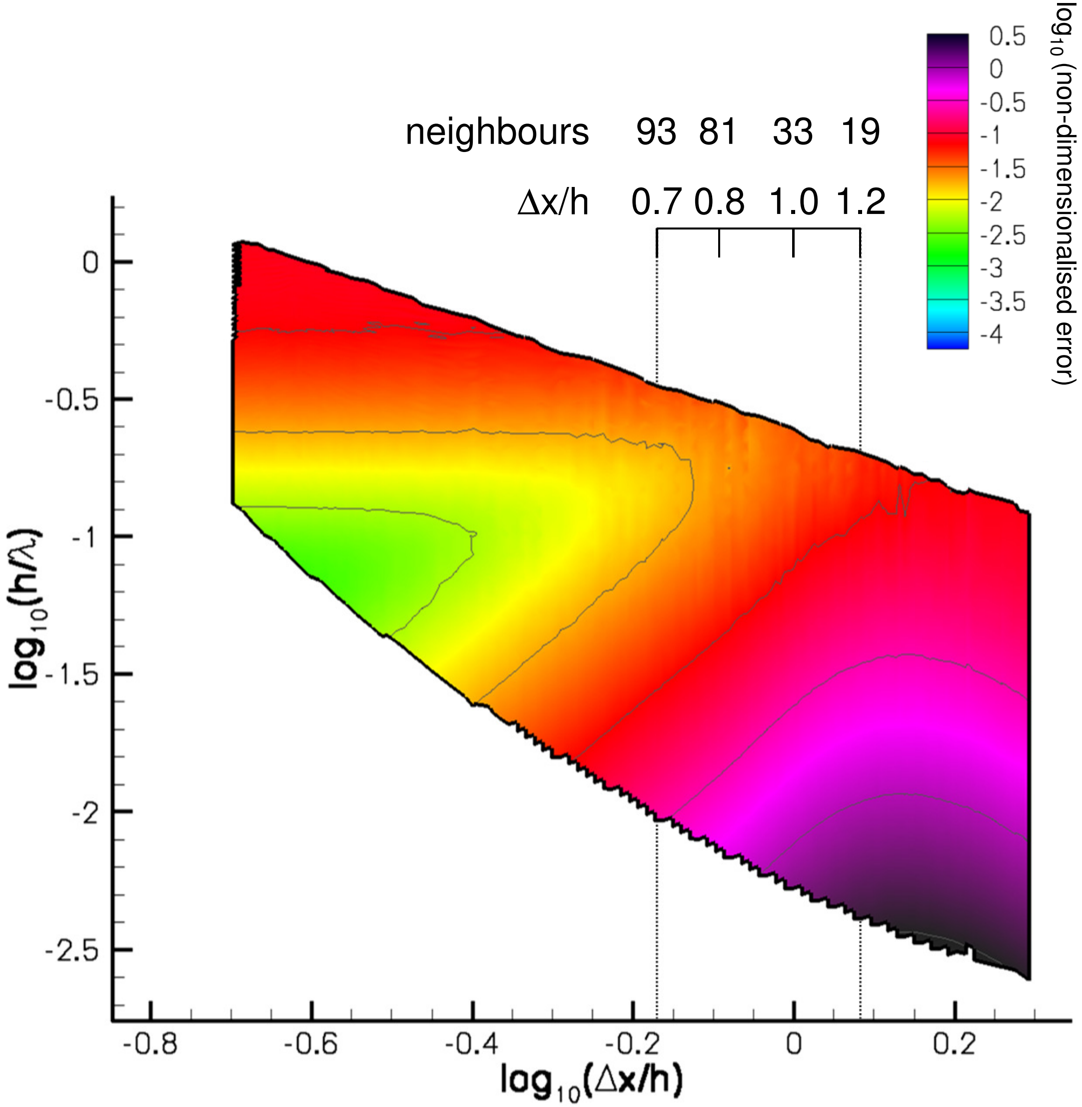


3D standard SPH

$\sigma/\Delta x = 0.2$

(high disorder)





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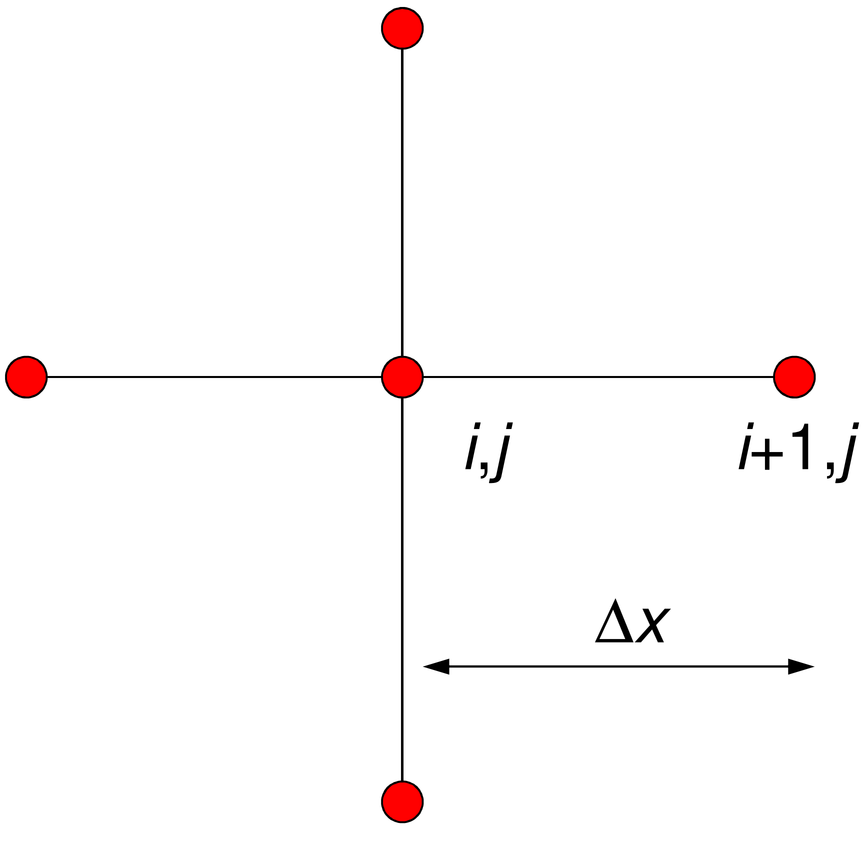
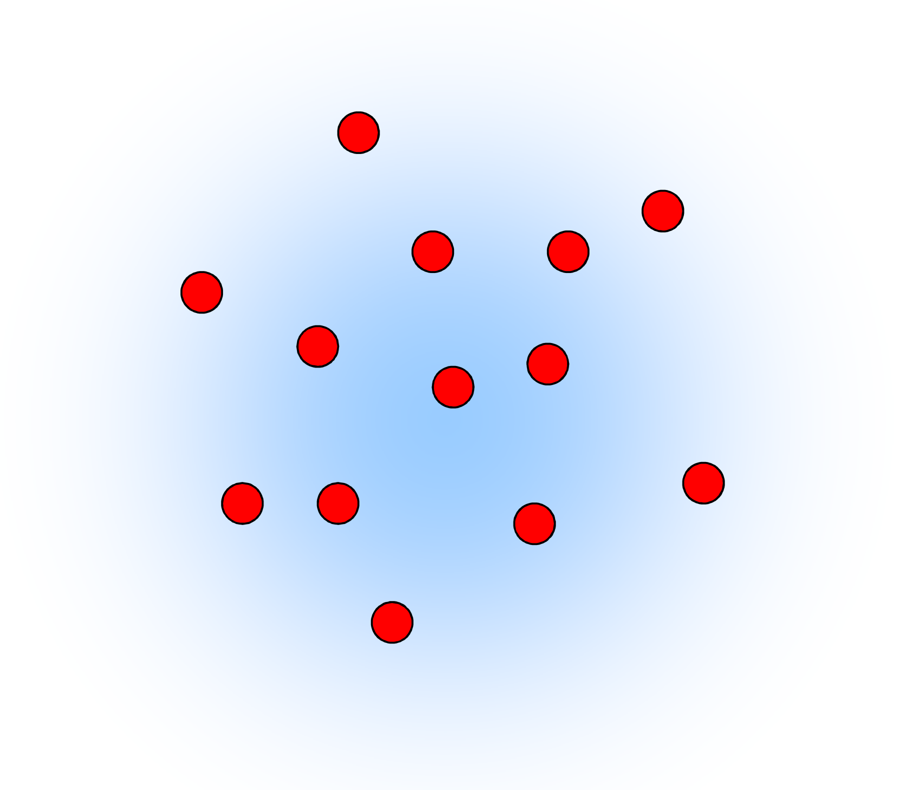
Stencils

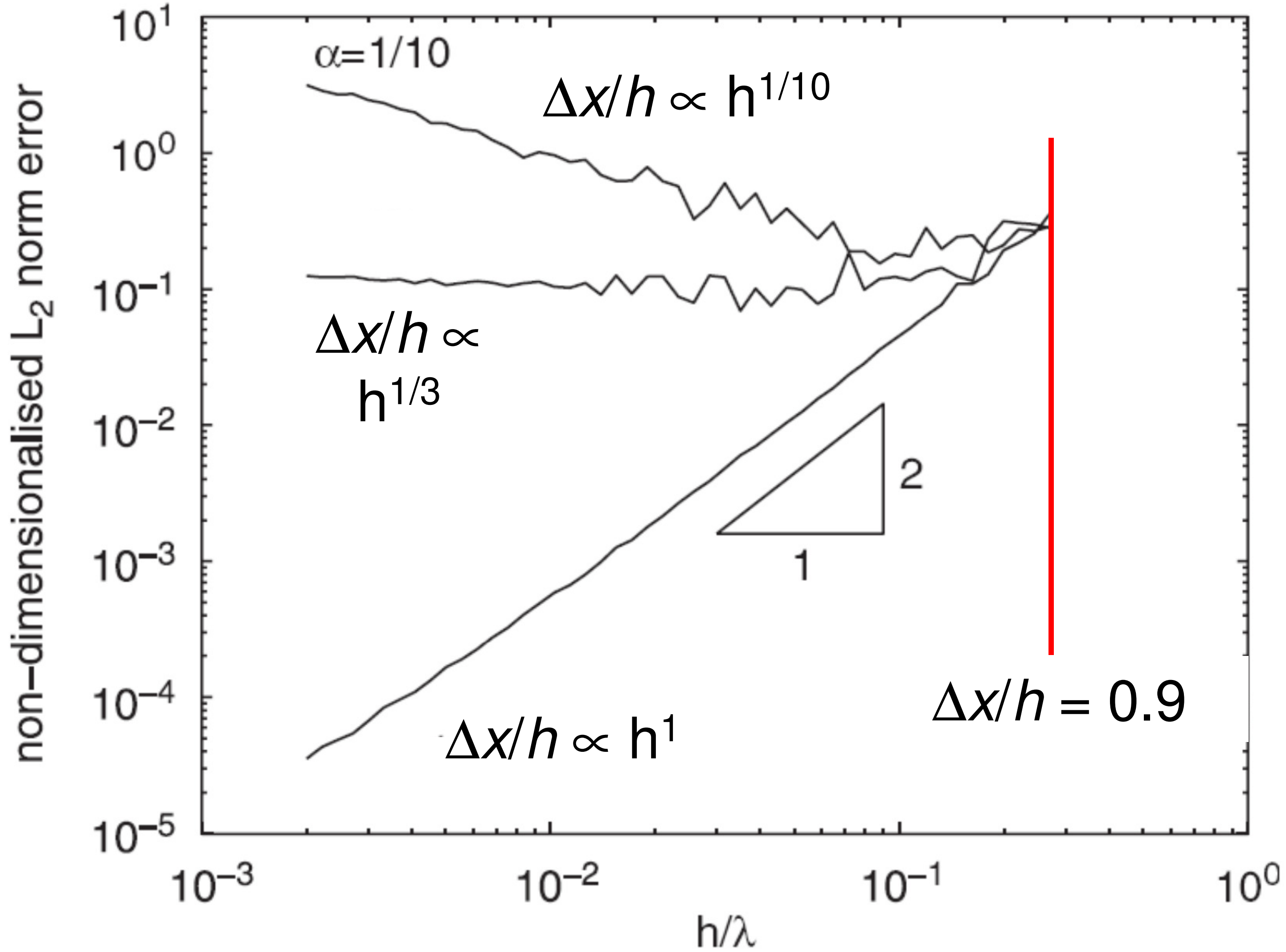


classical finite difference



SPH

Tuning $\Delta x/h$ and h/λ together



Context

Classical "second order" finite difference and finite volume methods are nearly always analysed on uniform meshes. Performance is degraded on non-uniform meshes.

– e.g. Turkel (1986)

"Order of accuracy isn't everything."

– Leveque (2004)

Second derivatives

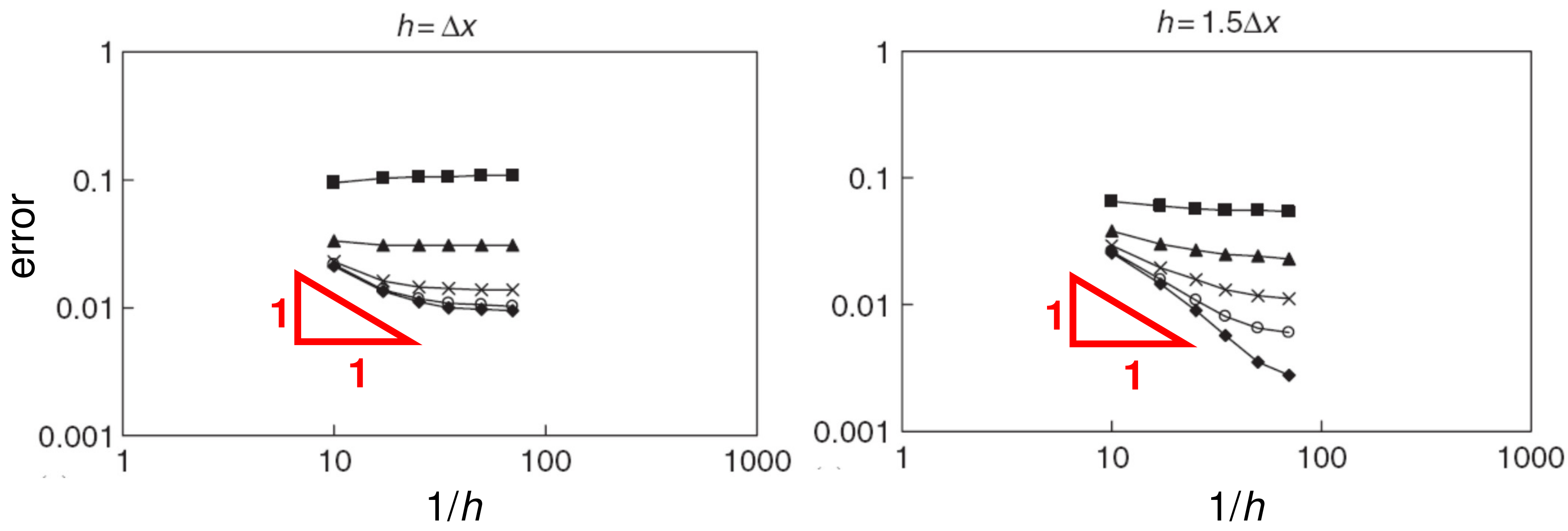
Popular form for computing viscous stress:

$$\nabla^2 A\Big|_a = \sum_b (A_b - A_a) \frac{\mathbf{x}_b - \mathbf{x}_a}{\left|\mathbf{x}_b - \mathbf{x}_a\right|^2} \bullet \nabla W_{ab} \frac{m_b}{\rho_b}$$

Conserves linear and angular momentum

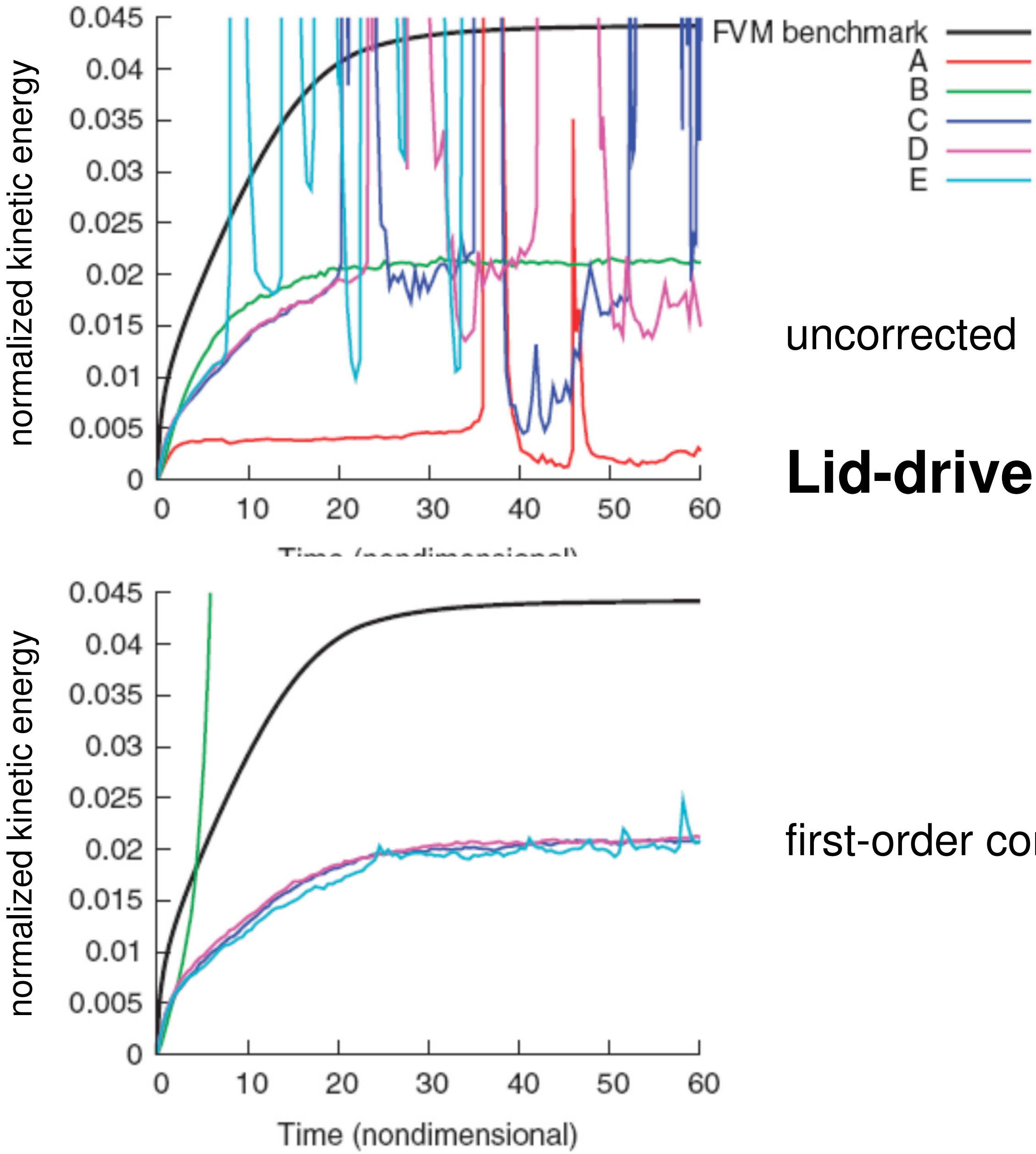
Relies on $(\mathbf{x}_b - \mathbf{x}_a) \parallel \nabla W_{ab}$ – not true for corrected kernels

Error in viscous flow models



Graham and Hughes (2007)

Accuracy of viscous flow models



uncorrected

Lid-driven cavity at Re_L = 1000

Basa *et al*. (2008)

first-order consistent

An alternative view

Lagrangian mechanics (Hamiltonian) – Price

$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} \cong -\sum_b A(x_b)\frac{\partial W(x_b - x_a)}{\partial x_b}\Delta x_b$$

Lagrangian of the particle set

$$L = \sum_b m_b\left[\frac{1}{2}v_b^2 - u(\rho, s)\right]$$

The $+\frac{p}{\rho^2}$ form emerges naturally

The only numerics in the proof is the density estimate

This is a system of particles – SPH is incidental

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"Why a bad derivative leads to good derivatives"

Price (2009)

- The $+\frac{p}{\rho^2}$ form of the momentum equation emerges naturally from the Lagrangian – it is special

- Interparticle forces are always repulsive (while *p*>0)

- Particles tend towards "regular" distributions

Conclusions

Convergence requires **consistency**, **conservation**, **stability**

- Difficult to combine conservation and consistency
- Absolute convergence is elusive
- Particle “disorder” is still poorly understood

References and further reading

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References and further reading