Conservative Reproducing Kernel Smoothed Particle Hydrodynamics for Solids

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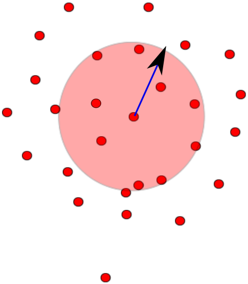
A quick reminder how (A)SPH and related meshless methods work.

- The physics variables (m_i, v_i^α, $S_i^{\alpha\beta}$, ...) are defined at an arbitrary set of points in space.
- These points move with the material velocity, arbitrarily reconnecting with new neighbors.
- Each point has an associated resolution/smoothing scale h_i.
  - h_i defines the set of neighbors point i interacts with.
- A basis function (or interpolation kernel) $W(r, h)$ is used to relate quantities between points.
- (A)SPH formalism describes the continuous representation of the nodal variables and their spatial gradients.



So what's wrong with SPH?

- SPH is based on a simple interpolation theory

$$\langle f(x)\rangle_{\mathrm{SPH}} = \int_{x'} dx'\, \mathrm{f}(x') W\big(x - x', h(x')\big) \approx \sum_j \frac{m_j}{\rho_j} F_j W(x - x_j, h_j)$$

  - W is the interpolation kernel, generally a cubic spline.
  - Assumes the normalization $\int_{x'} dx' W(x - x', h(x')) = 1$.
  - However, $\sum_j m_j/\rho_j W(x - x_j, h_j) \approx 1$.
    - For disordered points or near surfaces this approximation can be off by a factor of 2 or more.
- Because of this lack of consistency SPH interpolation is not zeroth order consistent, i.e., even a constant function will not be interpolated exactly.

Reproducing Kernels allow exact reproduction of functions.

- In the late 90's Reproducing Kernels (RK) were proposed as an enhanced form of SPH interpolation.[1]
  - Posit a corrected kernel (to linear terms) of the form

$$\langle f(x) \rangle_{\mathrm{RK}} = \sum_j V_j F_j \mathcal{W}_j^R, \qquad \mathcal{W}_j^R \equiv \left(A_i + B_i^\beta x_{ij}^\beta \right) W_j$$

  - Solve for (A_i, B_i^α) by requiring

$$\sum_j V_j \mathcal{W}_j^R = 1 \qquad\qquad \sum_j V_j x_{ij}^\alpha \mathcal{W}_j^R = 0$$

- After some algebra we find

$$A_i = \left[m_0 - \left(m_2^{-1} \right)^{\alpha\beta} m_1^\beta m_1^\alpha \right]^{-1} \qquad\qquad B_i^\alpha = - \left(m_2^{-1} \right)^{\alpha\beta} m_1^\beta$$

where

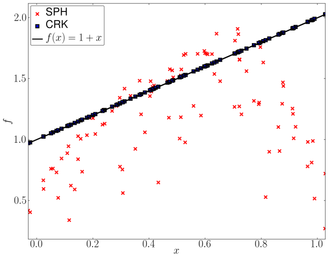
$$m_0 \equiv \sum_j V_j W_j, \qquad m_1^\alpha \equiv \sum_j x_{ij}^\alpha V_j W_j, \qquad m_2^{\alpha\beta} \equiv \sum_j x_{ij}^\alpha x_{ij}^\beta V_j W_j$$

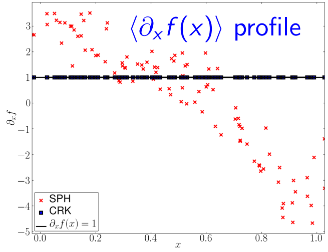
[1] Liu, Jun, and Zhang 1995; Liu, Jun, Li, et al. 1995.

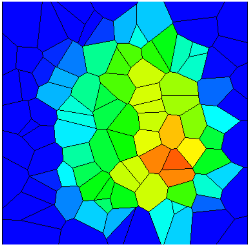
Interpolation and gradients with RK are much more accurate.

- We randomly place points in the box $(x, y) \in ([0,1],[0,1])$ and sample the function $f(x) = 1 + x$.
  - SPH shows the greatest errors along the boundaries.
  - RK interpolates the function and its gradient to round-off.

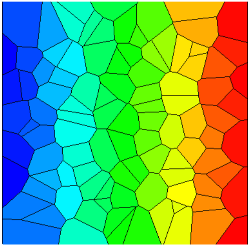
$\langle f(x) \rangle$ profile







$\langle f(x) \rangle$ SPH



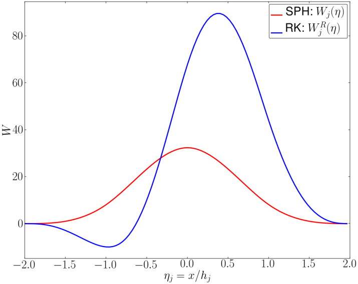
$\langle f(x) \rangle$ RK

So why haven't RK based methods supplanted SPH?

- Reproducing kernel interpolation makes enforcing conservation more difficult.
- The ordinary SPH momentum equation is

$$\frac{Dv_i^\alpha}{Dt} = -\sum_j m_j \left[\left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \partial^\alpha W_{ij} + \Pi_{ij}^{\beta\alpha} \partial^\beta W_{ij} \right]$$

- Implies $F_{ij}^\alpha = -F_{ij}^\alpha$ so long as $\partial^\alpha W_{ij} = -\partial^\alpha W_{ji}$.
- $\mathcal{W}_j^R$ breaks this symmetry because (A_i, B_i^α) are unique to each point: $\implies$ loss of rigorous conservation!
- RK methods to date have largely ignored this problem.



The standard reproducing kernel momentum equation.

- A typical RK discretization for the momentum equation directly employs the simple RK gradient operator

$$\frac{Dv_i^\alpha}{Dt} = -\rho_i^{-1} \partial^\beta \sigma^{\alpha\beta} = \rho_i^{-1} \sum_j V_j \sigma_j^{\alpha\beta} \partial^\beta \mathcal{W}_j^R$$

- Does not manifestly conserve linear momentum.
- Authors counting on higher accuracy of the differencing to keep the momentum error under control.[2]
- Most RK applications have been in low-energy solid modeling (tool cutting, bending beams, etc.)
  - This approach fairly successful for such applications.
- The lack of conservation is a weakness for strong shock/high energy applications however.

[2] Bonet and Kulasegaram 2000; Bonet, Kulasegaram, and Rodriguez-Paz 2004.

A conservative form of the momentum equation.

- We can derive an explicitly conservative form of the momentum equation by returning to the basic flux conservation equations convolved with volumetric integrals of the RK basis functions.
- Dilts demonstrates this procedure in the derivations of MLSPH[3].
- We derive this form in the context of RK interpolation theory.[4]

$$m_i \frac{Dv_i^\alpha}{Dt} = -\frac{1}{2} \sum_j V_i V_j \left\{ \left(\sigma_i^{\alpha\beta} + \sigma_j^{\alpha\beta}\right) \left(\partial^\beta \mathcal{W}_j^R - \partial^\beta \mathcal{W}_i^R\right) - \left(Q_i + Q_j\right) \left(\partial^\alpha \mathcal{W}_j^R - \partial^\alpha \mathcal{W}_i^R\right) \right\}$$

- Note $F_{ij} = -F_{ji}$, so we have restored exact conservation of linear momentum.
- This relation forms the core of Conservative Reproducing Kernel Smoothed Particle Hydrodynamics (CRKSPH).

[3] Dilts 2000.

[4] Frontire et al. 2015, in preparation.

The CRKSPH evolution equations.

- The remaining evolution equations (appropriate for solids) are

$$\frac{D\rho_i}{Dt} = -\,\rho_i \partial^\alpha v_i^\alpha \qquad \leftarrow \text{Potential weakness!}$$

$$\partial^\beta v_i^\alpha = \sum_j V_j \left(v_j^\alpha - v_i^\alpha\right) \partial^\beta \mathcal{W}_j^R$$

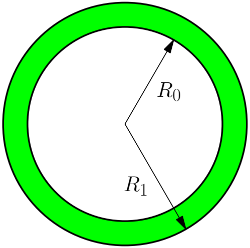
$$m_i \frac{D\varepsilon_i}{Dt} = \frac{1}{2} \sum_j V_i V_j \left(\sigma_j^{\alpha\beta} + Q_j \delta^{\alpha\beta}\right) \left(v_i^\beta - v_j^\beta\right) \left(\partial^\alpha \mathcal{W}_j^R - \partial^\alpha \mathcal{W}_i^R\right)$$

- At the end of each step the specific thermal energy ε_i is evolved using the same compatible discretization derived for SPH.[5]
- CRKSPH manifestly conserves mass, linear momentum, and total energy to machine precision.

[5] Owen 2014.

Test case: the Verney imploding shell.

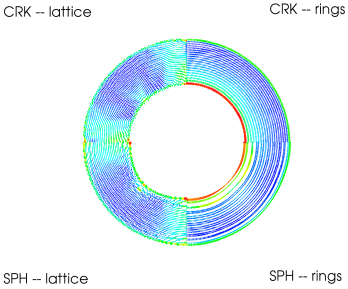
- The classic "stopping shell" test problem.[6]
- A cylindrical shell of Be is given an initial inward radial velocity profile such that all the kinetic energy will be converted via plastic work to internal energy at a known final inner radius.
  - Initial radii: $R_0 = 8$cm, $R_1 = 10$cm
  - Final expected inner radius: $r_0 = 4$cm
  - Osborne equation of state
  - Constant shear modulus and yield strength
  - Analytic solution assumes material is incompressible and follows shockless evolution.
- Initial conditions as in Howell & Ball (2002).
- It is important to use the ellipsoidal sampling of ASPH, as radial and azimuthal spacing of the points changes anisotropically!

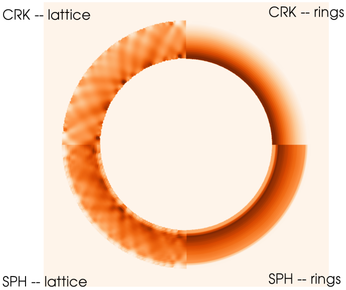


[6] Verney 1968; Howell and Ball 2002.

Cylindrical Verney implosion: point distributions, the choice of sampling volumes, and plastic strains.

- It is interesting to examine how this problem behaves with different methods of initializing the points:
  - Points arranged in rings of equal radial and azimuthal steps.
  - Points on a clipped lattice – antithetical to the physics geometry.





H

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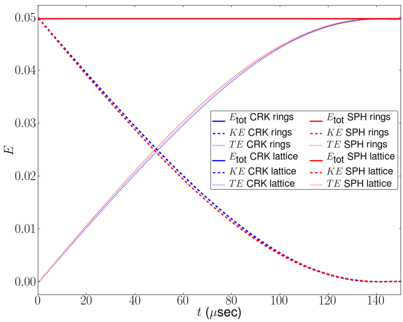
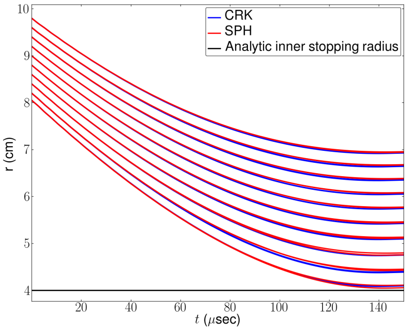
The energy and evolution of the radii match our expectations for the 2D Verney implosion.

- In all cases ($n_r \in [10, 20, 40, 80]$) the energy budgets show the expected conversion of kinetic to thermal energy via plastic work.
- Binning the points in radial shells and following the mass averaged radii histories is also nearly indistinguishable.



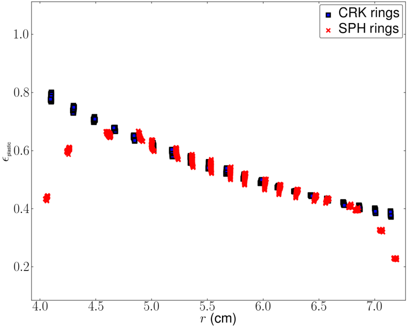
Energy evolution



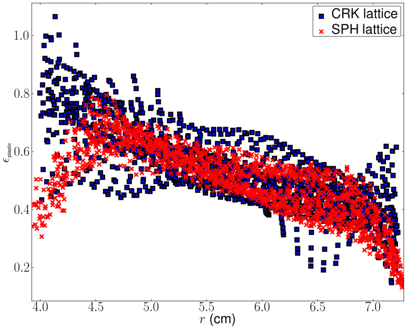
Mass averaged radii histories

Snapshots of the radial plastic strain profiles are more revealing.

- Radial profiles at $t = 150\mu$sec.
- The surface error in the SPH calculation is evident from the falloff of $\epsilon_{\text{plastic}}$ near the surfaces.
- Scatter due to the enhanced stresses launched from the rough surface in clipped lattice.
  - More pronounced in CRK.



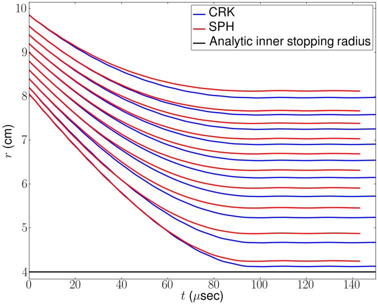
Seeded on rings

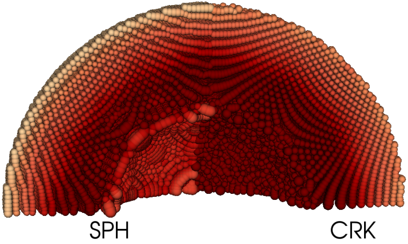


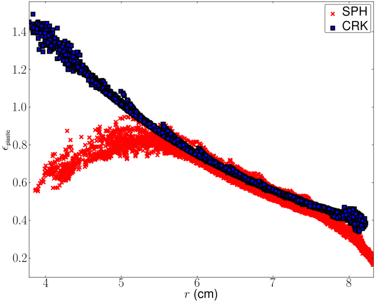
Seeded on clipped lattice

3D Verney implosion calculations tell a similar story.

- We show here a low-resolution 3D example ($n_r = 10$, seeded with clipped lattice).
- This investigation still in progress:
  - Go to higher resolutions.
  - Try using our icosahedral shells point generator.

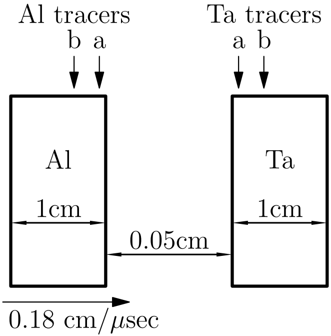






A flyer plate test allows us to examine strong shock behavior.

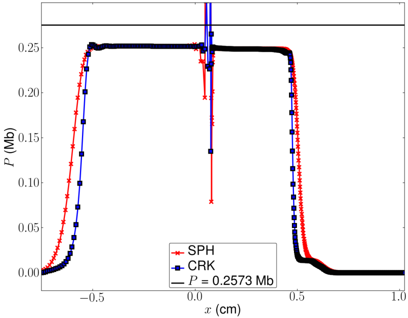
- This is an idealized flyer plate problem suggested by Wayne Weseloh and Fady Najjar.[7]
- An Al flyer plate impacts a Ta target at 0.18 cm/μsec.
  - Employs a simplified Gruneisen equation of state (function of density only).
  - Steinberg-Guinan strength model.
- Analytic solution predicts post-shock pressure of $P_{\text{shock}} = 0.2753$Mb.
- An interesting test of the SPH surface problem, as materials start out separated but then collide.

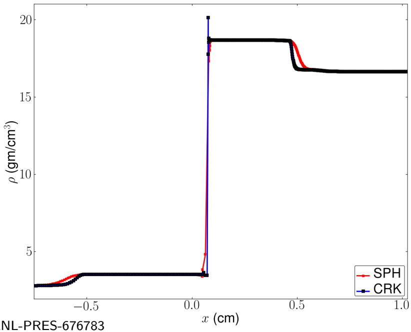


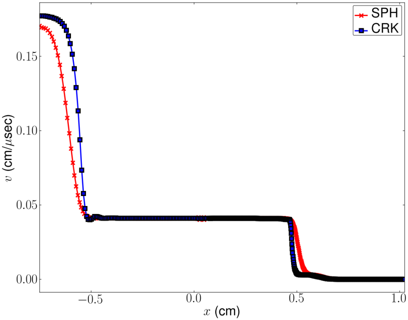
[7] Weseloh and Najjar 2011.

Flyer plate profiles at $t = 1.5\mu$sec.

- CRK shows sharper transitions.
- Largest errors at collision point.
- Both methods slightly underestimate the post-shock pressure.
- Likely due to density equation.

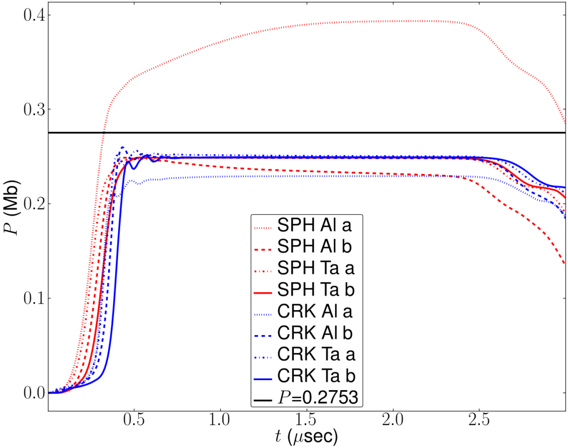






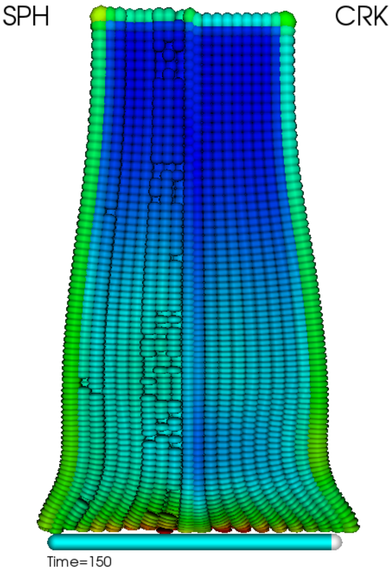
Flyer plate pressure histories.

- The tracers in the Al at the collision surface show the largest deviations.
- In all cases SPH has larger errors in the pressure history.
- In the interior of the plates both methods converge to the same underestimate of the analytic solution.



The Taylor anvil.

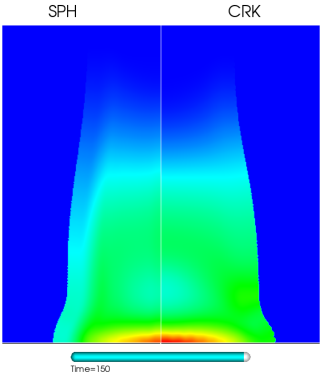
- Based on an experiment published by Eakins & Thadhani[8].
- Consists of a 7.5cm long, 1cm radius cylindrical rod of Cu impacting a wall at 205 m/sec.
- Though there is no analytic solution, the Taylor anvil is useful as
  - a stability test of the numerical model;
  - a check of strength and yield models.
- Modeled here as full cylinders, which for visualization purposes are clipped to quadrants.



[8] Eakins and Thadhani 2006.

Plastic strain evolution in the Taylor anvil.

- Both SPH and CRKSPH model this problem reasonably.
- CRK sees more plastic deformation in the core of the foot, a bit more extension of the foot, and slightly more compression of the rod length.
- We can clearly see the SPH surface error in the plastic strain calculation.
- CRKSPH seems to treat the strain consistently out to the surface.

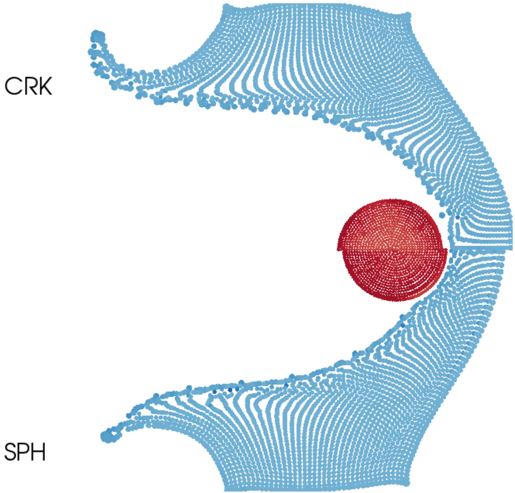


Slice of $\epsilon_{\text{plastic}}$

Conclusions and future directions.

- CRKSPH improves on the weaknesses of SPH while maintaining its strengths.
  - Common strengths: conservative, meshfree, simple to understand and implement, Lagrangian, ...
  - CRK strengths: Accuracy, consistency.
  - Remaining weaknesses: need better mass density relation, filter for parasitic modes.
- CRKSPH seems as good or better than ordinary SPH thus far.
- Future directions:
  - We are experimenting with ideas for a better mass density equation.
  - Also looking at some filtering ideas to treat parasitic modes/"tensile error".
  - Is it worth going to higher-order sampling than linear? RK formalism can be extended to an arbitrary order.
  - Damage modeling for fracture and failure (already experimentally implemented).
- See Cody Raskin's upcoming talk for the fluid limit!

Questions?



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