Chasing a Ghost: One Fool's Quest for Perfection in SPMHD

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Research Interests

- I am interested in the **pedantic numerical details of SPH**.
- One of my key research areas is in SPMHD – **Smoothed Particle Magnetohydrodynamics**.

Modern State of SPMHD

Smoothed Particle Magnetohydrodynamics

- From the inception of SPH, there was unbridled optimism about performing MHD with SPH.

".. magnetic fields may be included without difficulty.."

Gingold & Monaghan (1977)

Smoothed Particle Magnetohydrodynamics

- In some respects, **Joe was right!** It is straightforward.
- Take the induction equation for evolving B forward in time,

$$\frac{\mathrm{d}\mathbf{B}}{\mathrm{d}t} = -\left(\mathbf{B}\cdot\nabla\right)\mathbf{v} + \mathbf{B}\left(\nabla\cdot\mathbf{v}\right)$$

- and apply standard SPH to it.
- Has some nice properties – namely, Galilean invariance.

$$\frac{\mathrm{d}\mathbf{B}_a}{\mathrm{d}t} = -\frac{1}{\Omega_a\rho_a}\sum_b m_b\left[\mathbf{v}_{ab}(\mathbf{B}_a\cdot\nabla_a W_{ab}(h_a)) - \mathbf{B}_a(\mathbf{v}_{ab}\cdot\nabla_a W_{ab}(h_a))\right]$$

Smoothed Particle Magnetohydrodynamics

- Can solve for conservative equations of motion.

$$\frac{\mathrm{d}\mathbf{v}_a}{\mathrm{d}t} = -\sum_b m_b \left[\frac{P_a}{\Omega_a \rho_a^2}\nabla_a W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2}\nabla_a W_{ab}(h_b)\right] - \frac{1}{2\mu_0}\sum_b m_b \left[\frac{B_a^2}{\Omega_a \rho_a^2}\nabla_a W_{ab}(h_a) + \frac{B_b^2}{\Omega_b \rho_b^2}\nabla_a W_{ab}(h_b)\right] + \frac{1}{\mu_0}\sum_b m_b \left[\frac{\mathbf{B}_a}{\Omega_a \rho_a^2}\mathbf{B}_a \cdot \nabla_a W_{ab}(h_a) + \frac{\mathbf{B}_b}{\Omega_b \rho_b^2}\mathbf{B}_b \cdot \nabla_a W_{ab}(h_b)\right]$$

- And we can identify these terms directly in the stress tensor.
- Have magnetic pressure and magnetic tension, specifically.

$$\frac{\mathrm{d}v^i}{\mathrm{d}t} = \frac{1}{\rho}\frac{\partial S^{ij}}{\partial x^j} \qquad S^{ij} = -\delta^{ij}\left(P + \frac{B^2}{2\mu_0}\right) + \frac{B^i B^j}{\mu_0}$$

Magnetic Monopoles

- Of course, this does not place any constraint on the divergence of B.
- This must be true: $\nabla \cdot \mathbf{B} = 0$
- But is it in a simulation?
- Must do some extra work to guarantee this!

Magnetic Monopoles

- The effects of non-zero divergence of B are problematic.

- The magnetic tension in the stress tensor can be expanded to give:

$$B^i B^j \longrightarrow (\mathbf{B} \cdot \nabla)\mathbf{B} + \mathbf{B}(\nabla \cdot \mathbf{B})$$

- In nature, the second term is zero. Adding a zero doesn't matter.
- In simulation, the second term may be non-zero. It does matter!
- Can cause unphysical clumping of particles (exaggerated tension).

Magnetic Monopoles

- The fix for this is straightforward.
- Subtract out the unphysical force!

$$-\mathbf{B}(\nabla \cdot \mathbf{B}) = -\mathbf{B}_a \sum_b m_b \left(\frac{\mathbf{B}_a}{\Omega_a \rho_a^2} \cdot \nabla_a W_{ab}(h_a) + \frac{\mathbf{B}_b}{\Omega_b \rho_b^2} \cdot \nabla_a W_{ab}(h_b) \right)$$

- Yields a **robust, numerically stable** solution.
- But is **no longer momentum conserving.**
- However, if DivB = 0, this non-conservation is (mostly) a non-issue.

Magnetic Monopoles

- The key question in SPMHD is: how to uphold $\nabla \cdot \mathbf{B} = 0$?

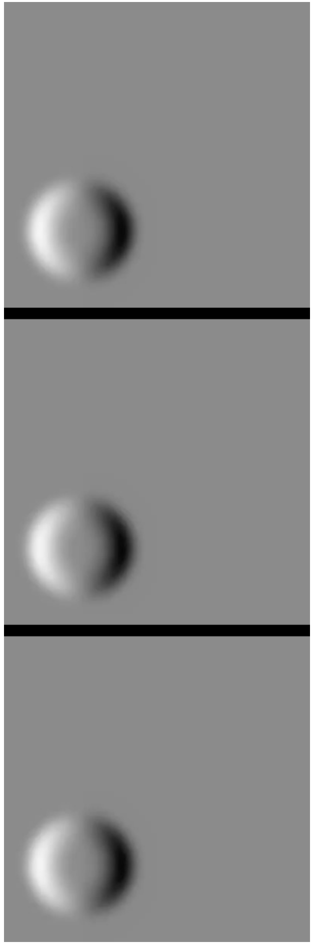
Constrained Divergence Cleaning

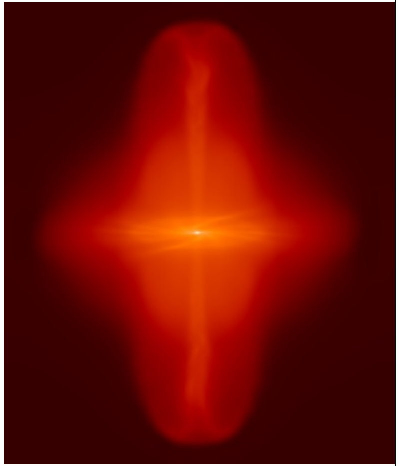
- One of my key contributions in this area is **Constrained Hyperbolic/Parabolic Divergence Cleaning**. (Dedner et al, 2002; Tricco & Price, 2012; Tricco, Price & Bate, 2016)

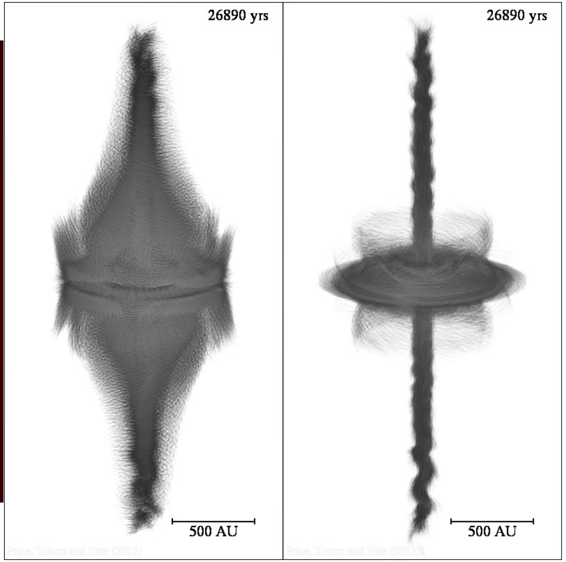
- Divergence errors are spread over a larger volume and damped.

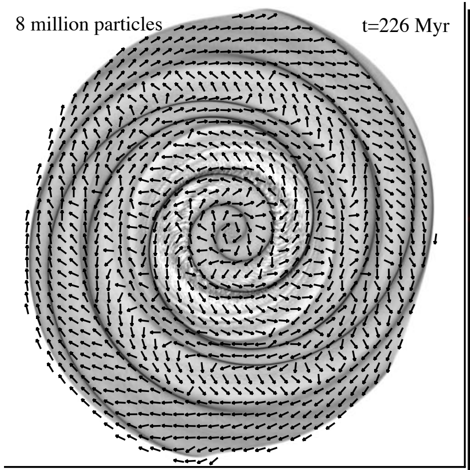
$$\frac{\mathrm{d}\mathbf{B}}{\mathrm{d}t} = (\mathbf{B}\cdot\nabla)\mathbf{v} - \mathbf{B}(\nabla\cdot\mathbf{v}) - \nabla\psi$$

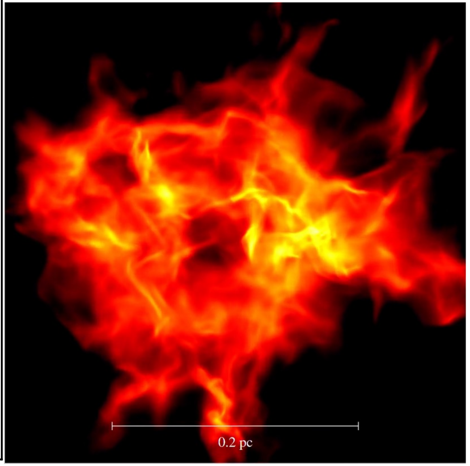
$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = -c_{\mathrm{h}}^2\nabla\cdot\mathbf{B} - \frac{\psi}{\tau}$$

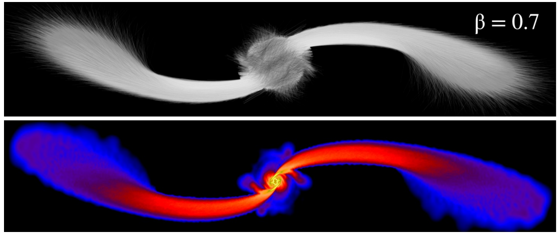


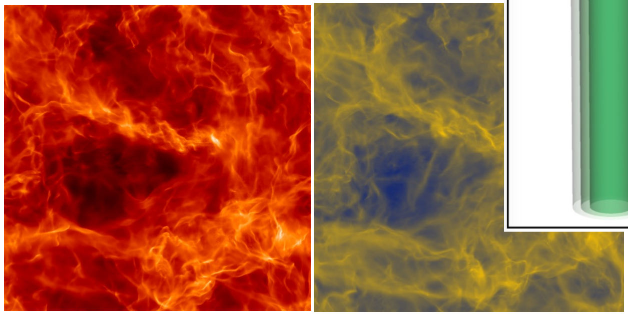


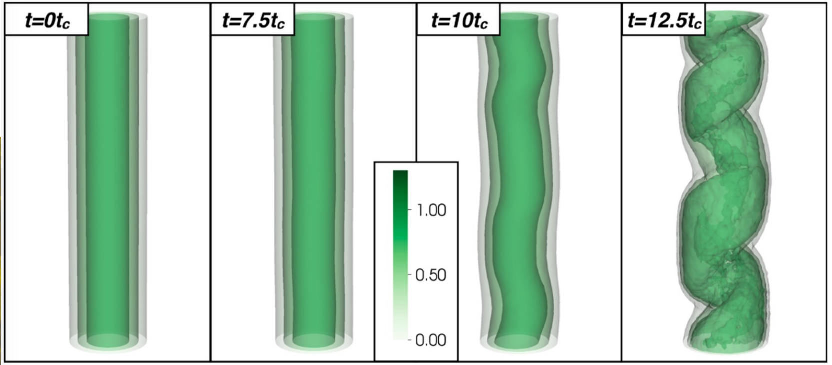












Price, Tricco & Bate (2012); Dobbs, Price, Pettitt, Bate, Tricco (2016); Bonnerot et al (2017); Liptai et al (2017); Tricco Price & Federrath (2016); Vela Vela et al (2019)

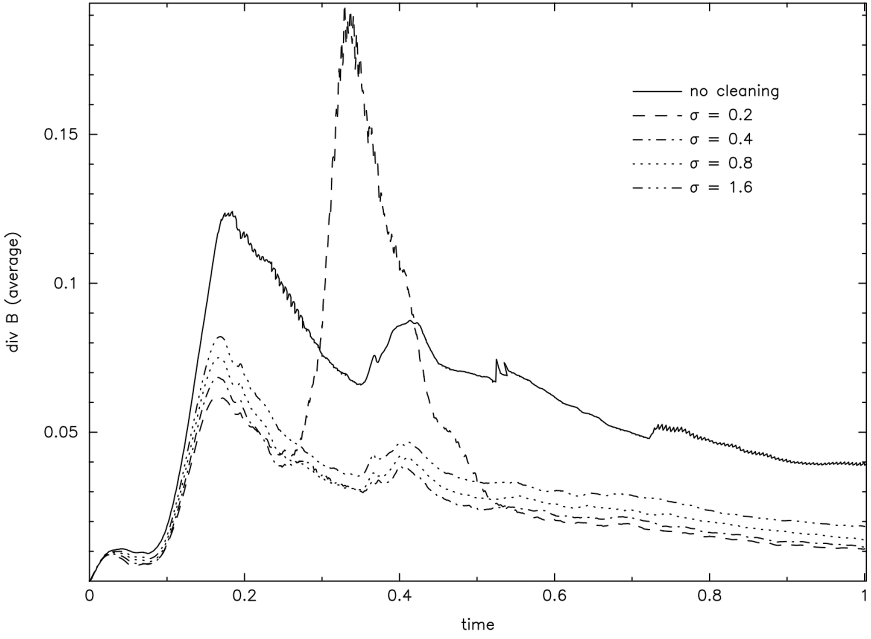
And many more on the MRI, colliding clouds, the Milky Way, star formation, star cluster formation, disc formation by Dobbs, Wurster, Bate, Wissing, Shen, etc

(Un)-Constrained Divergence Cleaning

- *"The optimal cleaning is obtained with σ ∼ 0.4–0.8 (dot–dashed, dotted lines), although the reduction in the divergence error given by the* ***hyperbolic cleaning is comparatively small."***

- *"The results using the hyperbolic/parabolic cleaning with σ = 0.2 (dashed line)* ***can in fact increase the divergence error*** *over the results with no divergence cleaning (solid line)."*

Price & Monaghan (2005)



Constrained Divergence Cleaning

- To build this into SPMHD, we approached this from the perspective of **energy conservation**.

- Energy is transferred between B and the cleaning field.
- This transfer must balance. Otherwise spurious energy is created.
- (This may lead to an increase in divergence error, as found in PM05!)

Constrained Divergence Cleaning

- Can determine the energy stored in the cleaning field. $e_\psi \equiv \dfrac{\psi^2}{2\mu_0\rho c_h^2}$
- Energy transferred between the magnetic and cleaning fields must balance.

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \sum_a m_a \left[\frac{\mathbf{B}_a}{\mu_0\rho_a} \cdot \left(\frac{\mathrm{d}\mathbf{B}_a}{\mathrm{d}t}\right)_\psi + \frac{\psi_a}{\mu_0\rho_a c_h^2}\frac{\mathrm{d}\psi_a}{\mathrm{d}t} \right] = 0$$

- Solving the SPMHD cleaning equations yields very specific operator choices.
- Must use a **first-order accurate method for calculating divB**.
- And a **zeroth-order accurate method for the gradient of psi**.
- (This duality is seen in other contexts – e.g., pressure gradient, resistive SPMHD, etc)

Constrained Divergence Cleaning

- The original equations by Dedner et al (2002):

$$\frac{\mathrm{d}\mathbf{B}}{\mathrm{d}t} = (\mathbf{B}\cdot\nabla)\mathbf{v} - \mathbf{B}(\nabla\cdot\mathbf{v}) - \nabla\psi$$

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = -c_{\mathrm{h}}^2\nabla\cdot\mathbf{B} - \frac{\psi}{\tau}$$

- We showed that the correct set of equations, accounting for density variations and time-varying cleaning rates (c_h) are:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\psi}{c_{\mathrm{h}}}\right) = -c_{\mathrm{h}}(\nabla\cdot\mathbf{B}) - \frac{1}{\tau}\left(\frac{\psi}{c_{\mathrm{h}}}\right) - \frac{1}{2}\left(\frac{\psi}{c_{\mathrm{h}}}\right)(\nabla\cdot\mathbf{v})$$

Modern SPMHD

- Our constrained cleaning typically provides a **10x reduction in divergence error**, and keeps average **error around the ~1% level**.

Modern SPMHD

- Our constrained cleaning typically provides a **10x reduction in divergence error**, and keeps average **error around the ~1% level**.

- Our lesson is that SPH knows best.
- When creating numerical methods, trust SPH and do what it tells you do!
- Build your numerical equations to conserve energy and all your wildest dreams will come true!

The Future of SPMHD

Future SPMHD

- My goal is to create a truly **divergence-free** SPMHD.

Future SPMHD

- Divergence cleaning has unlocked many research areas.

- However, it is an approximate method.
- Divergence errors are continually being introduced and cleaned away.
- Steady state is (typically) around the 1% error level.

- Ideally, want a method that prevents divergence errors by construction!

Euler Potentials

- One approach to do just this is to use the Euler Potentials.

$$\boldsymbol{B} = \nabla\alpha_{\mathrm{E}} \times \nabla\beta_{\mathrm{E}}$$

$$\frac{\mathrm{d}\alpha_{\mathrm{E}}}{\mathrm{d}t} = 0$$

$$\frac{\mathrm{d}\beta_{\mathrm{E}}}{\mathrm{d}t} = 0$$

- Evolve the potentials, calculate B, then use SPMHD as normal.
- This works well! (sort of, Price & Bate, 2007/08/09; Price & Rosswog, 2006)

Euler Potentials

- The Euler Potentials do not live up to their potential.

- They cannot represent certain magnetic field configurations.
- Can represent toroidal or poloidal fields, but not both.
- Cannot create such complex fields during simulation.

- For example, simulations using the Euler Potentials do not see jets during protostar formation, which we do see in modern SPMHD simulations.

Vector Potential

- Formulating the magnetic field in terms of the Vector Potential is the next most logical choice.

$$\mathbf{B} = \nabla \times \mathbf{A}$$

- The divergence of the curl is zero. Guaranteed divergence-free magnetic field.

Vector Potential in SPMHD

- All we need to do is evolve the vector potential.

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B})$$

$$\frac{\partial \mathbf{A}}{\partial t} = \mathbf{v} \times (\nabla \times \mathbf{A}) + \nabla \phi,$$

$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} = \mathbf{v} \times (\nabla \times \mathbf{A}) + (\mathbf{v} \cdot \nabla)\mathbf{A} + \nabla \phi$$

- Choose a suitable gauge. $\phi = -\mathbf{v} \cdot \mathbf{A}$

$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} = -\mathbf{A} \times (\nabla \times \mathbf{v}) - (\mathbf{A} \cdot \nabla)\mathbf{v}$$

- Galilean invariant SPMHD equation!

$$\frac{\mathrm{d}\mathbf{A}_a}{\mathrm{d}t} = \frac{1}{\Omega_a \rho_a} \sum_b m_b (\mathbf{A}_a \cdot \mathbf{v}_{ab}) \nabla_a W_{ab}(h_a)$$

Vector Potential in SPMHD

- Evolve the vector potential and reconstruct the magnetic field (Price, 2010).

$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} = -\mathbf{A} \times (\nabla \times \mathbf{v}) - (\mathbf{A} \cdot \nabla)\mathbf{v}$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

$$\frac{\mathrm{d}\mathbf{A}_a}{\mathrm{d}t} = \frac{1}{\Omega_a \rho_a} \sum_b m_b (\mathbf{A}_a \cdot \mathbf{v}_{ab}) \nabla_a W_{ab}(h_a)$$

$$\mathbf{B}_a = \frac{1}{\Omega_a \rho_a} \sum_b m_b (\mathbf{A}_a - \mathbf{A}_b) \times \nabla_a W_{ab}(h_a)$$

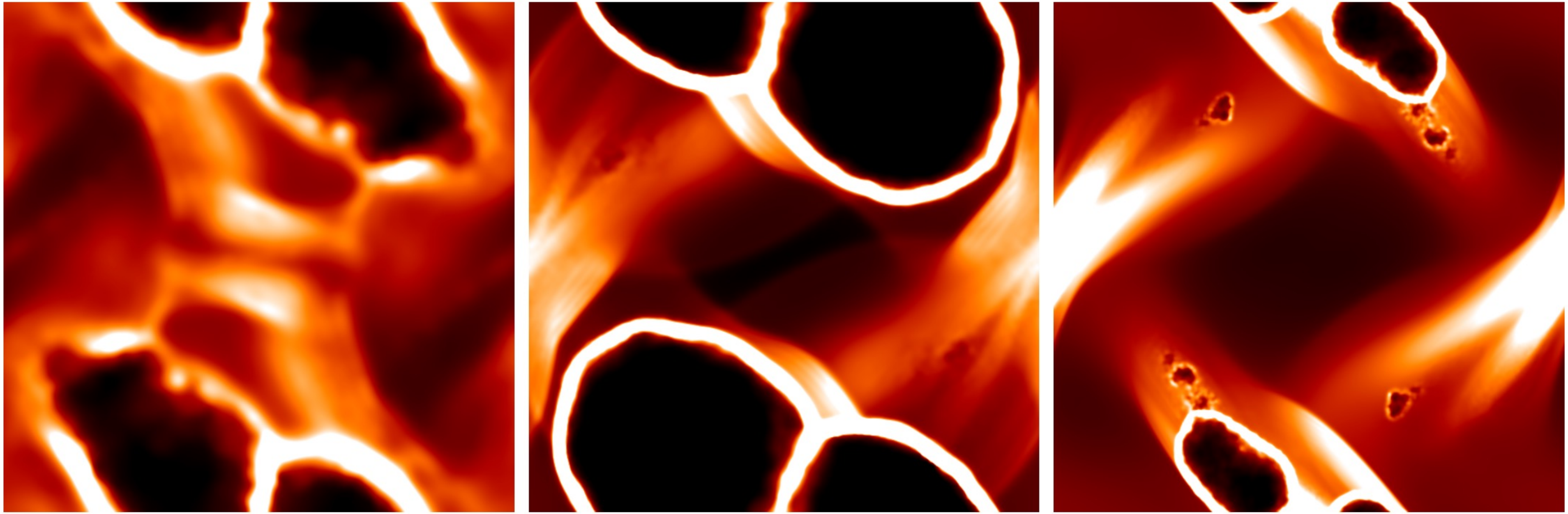
- Plug B into the SPMHD equations of motion. What could go wrong?

Orszag-Tang Vortex with Vector Potential

64 x 64 particles, t = 0.5

128 x 128 particles, t = 0.3

256 x 256 particles, t = 0.1975



Vector Potential in SPMHD

- This vector potential formulation is highly numerically unstable.

- Why?
- It does not conserve energy!
- The equations of motion were derived assuming the magnetic field was evolved according to the induction equation. We are not doing that.
- Instability therefore occurs and energy grows exponentially.

Vector Potential in SPMHD

- So the fix is to listen to SPH!
- Create the equations SPH wants us to create!
- Solve for the equations of motion in terms of the vector potential.

$$L_{\text{SPH}} = \sum_{b=1}^{N} m_b \left[\frac{1}{2} v_b^2 - u_b(\rho_b, s_b) - \frac{1}{2\mu_0} \frac{B_b^2}{\rho_b} \right]$$

- Conserve energy and all problems will be solved, right?

Vector Potential in SPMHD

- Price (2010) derived these equations.

$$\frac{\mathrm{d}\boldsymbol{v}_a}{\mathrm{d}t} = -\sum_b m_b \left(\frac{P_a - \frac{3}{2\mu_0} B_a^2}{\rho_a^2} + \frac{P_b - \frac{3}{2\mu_0} B_b^2}{\rho_b^2} \right) \nabla_a W_{ab}$$

$$- \frac{1}{\mu_0} \sum_b m_b \left\{ \left(\frac{\boldsymbol{B}_a}{\rho_a^2} + \frac{\boldsymbol{B}_b}{\rho_b^2} \right) \cdot [(\boldsymbol{A}_a - \boldsymbol{A}_b) \times \nabla] \right\} \nabla_a W_{ab}$$

$$- \sum_b m_b \left[\frac{\boldsymbol{A}_a}{\rho_a^2} \boldsymbol{J}_a \cdot \nabla_a W_{ab} + \frac{\boldsymbol{A}_b}{\rho_b^2} \boldsymbol{J}_b \cdot \nabla_a W_{ab} \right]$$

Pressure gradient +
Negative magnetic pressure

Kernel second derivative

Imposes inaccurate current density estimate

Vector Potential in SPMHD

- Measures had to be added to address all 3 components of the force.
  - Stabilize the negative pressure gradient.
  - High-order kernels to get a reasonable measure of the second derivative.
  - Use more accurate operators for the current density.
- Can simulate a shock tube, but that's about it.

- The 2D (not even 3D!) Orszag-Tang:
  - *"we are unable to produce a stable and accurate solution to the Orszag-Tang vortex using the consistent vector potential formulation."*

Vector Potential in SPMHD

- Daniel concludes with some gentle caution about the vector potential.

  - *"Perhaps the most useful aspect of this paper –* ***apart from acting as a warning to the reader intent on similar endeavours*** *– is the formulation of dissipative terms for the vector potential"*

  - *"leading us to conclude that use of* ***the vector potential is not a viable approach*** *for SPMHD."*

One Fool's Quest

- I have been studying the vector potential off and on for the past few years attempting to find any progress forward.

A New Hope?

- One initially promising venture was to formulate the vector potential in **integral form**.

$$\frac{\partial \mathbf{A}}{\partial t} = \mathbf{v} \times (\nabla \times \mathbf{A}) \quad \longrightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_V \mathbf{A}\mathrm{d}V = \int_v \mathbf{v} \times \mathbf{B}\mathrm{d}V + \int_{\partial V} \mathbf{A}\mathbf{v} \cdot \mathrm{d}S,$$

$$= \int_v \mathbf{v} \times \mathbf{B}\mathrm{d}V + \int_V \nabla_j (\mathbf{A}\mathbf{v}^j)\mathrm{d}V.$$

- Which discretized into SPMHD yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{A}_a}{\rho_a}\right) = \frac{\mathbf{v}_a \times \mathbf{B}_a}{\rho_a} + \frac{1}{\rho_a}\nabla_j (\mathbf{A}_a \mathbf{v}_a^j)$$

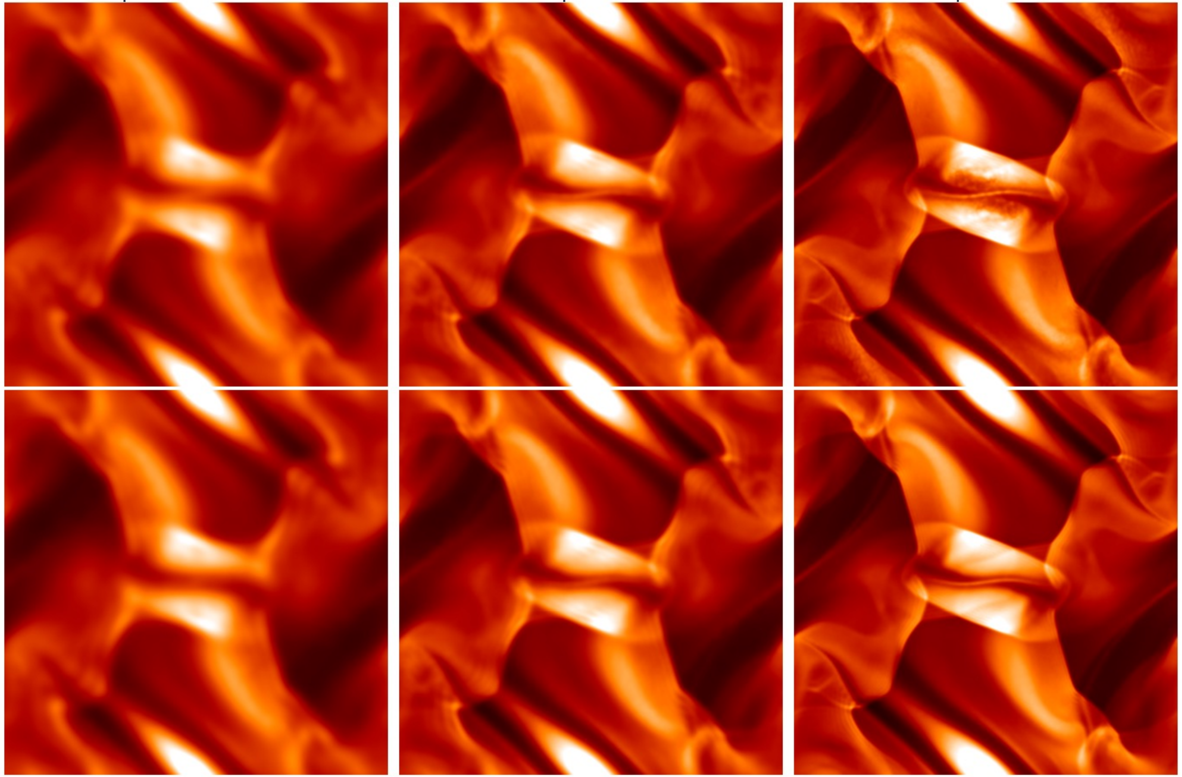
Integral Evolution of the Vector Potential

64 x 64 particles | 128 x 128 particles | 256 x 256 particles

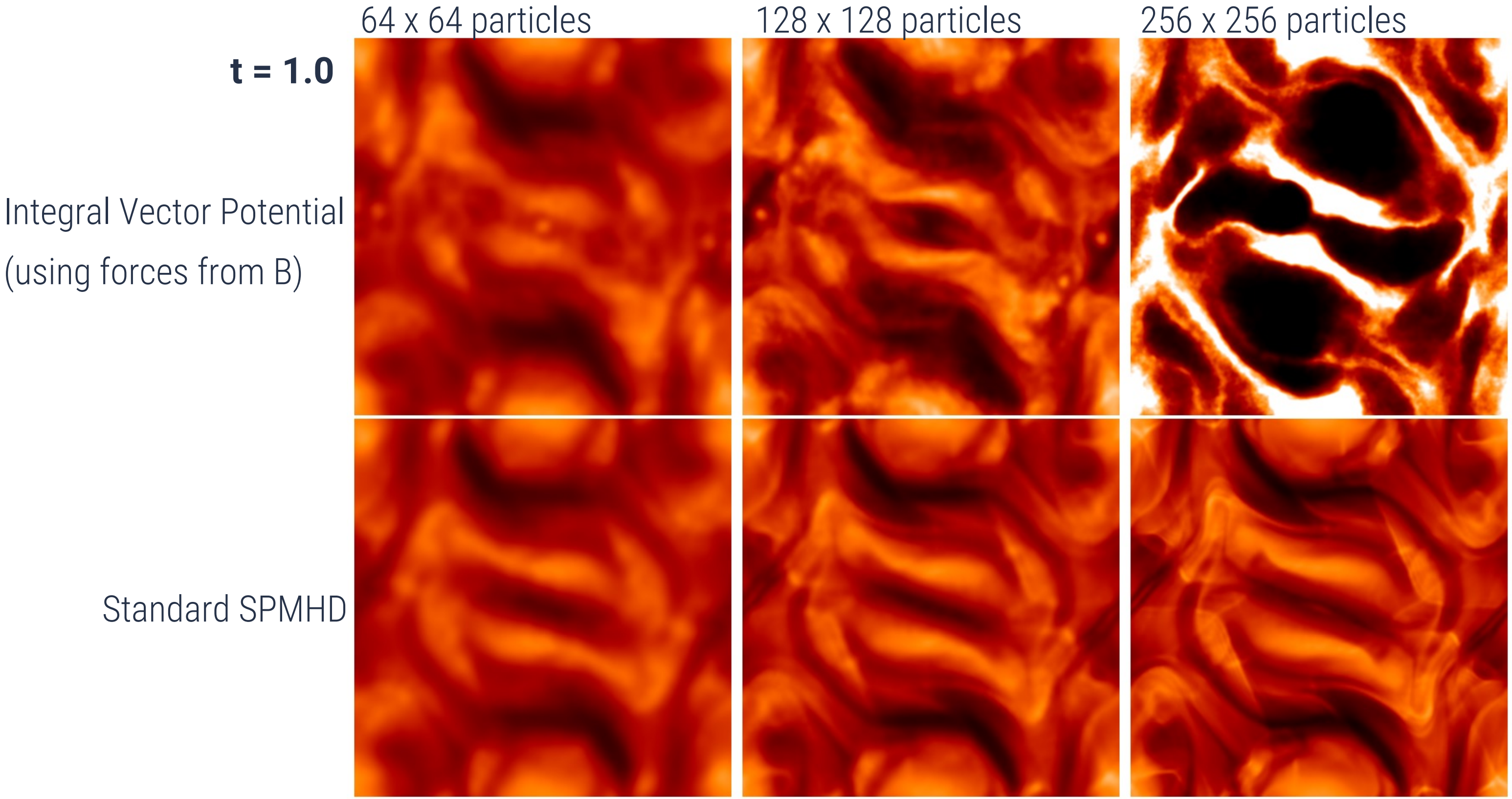
t = 0.5

Integral Vector Potential (using forces from B)

Standard SPMHD



Integral Evolution of the Vector Potential



Integral Evolution of the Vector Potential

- Evolving the vector potential with an integral approach helps!
- It is still numerically unstable, but can evolve the system longer before instability occurs.
- (Also this form is not Galilean invariant. Gauge choice may fix this?)
- Conclusion: Still not a panacea.

Energy Conservation

- A second avenue I have been investigating is to address the problems with the consistent formulation of the equations of motion.
- Goal: conserve energy!

$$
\begin{aligned}
\frac{\mathrm{d}\boldsymbol{v}_a}{\mathrm{d}t} = &-\sum_b m_b \left(\frac{P_a - \frac{3}{2\mu_0} B_a^2}{\rho_a^2} + \frac{P_b - \frac{3}{2\mu_0} B_b^2}{\rho_b^2} \right) \nabla_a W_{ab} \\
&- \frac{1}{\mu_0} \sum_b m_b \left\{ \left(\frac{\boldsymbol{B}_a}{\rho_a^2} + \frac{\boldsymbol{B}_b}{\rho_b^2} \right) \cdot \left[(\boldsymbol{A}_a - \boldsymbol{A}_b) \times \nabla \right] \right\} \nabla_a W_{ab} \\
&- \sum_b m_b \left[\frac{\boldsymbol{A}_a}{\rho_a^2} \boldsymbol{J}_a \cdot \nabla_a W_{ab} + \frac{\boldsymbol{A}_b}{\rho_b^2} \boldsymbol{J}_b \cdot \nabla_a W_{ab} \right]
\end{aligned}
$$

Energy Conservation

- But what can we do?

$$\frac{\mathrm{d}\boldsymbol{v}_a}{\mathrm{d}t} = -\sum_b m_b \left(\frac{P_a - \frac{3}{2\mu_0} B_a^2}{\rho_a^2} + \frac{P_b - \frac{3}{2\mu_0} B_b^2}{\rho_b^2} \right) \nabla_a W_{ab}$$

We are stuck with this. In theory, the rest of the terms contain part of the isotropic pressure.

$$- \frac{1}{\mu_0} \sum_b m_b \left\{ \left(\frac{\boldsymbol{B}_a}{\rho_a^2} + \frac{\boldsymbol{B}_b}{\rho_b^2} \right) \cdot \left[(\boldsymbol{A}_a - \boldsymbol{A}_b) \times \nabla \right] \right\} \nabla_a W_{ab}$$

Arises solely by the choice of the functional form of the kernel. Independent of how A is evolved.

$$- \sum_b m_b \left[\frac{\boldsymbol{A}_a}{\rho_a^2} \boldsymbol{J}_a \cdot \nabla_a W_{ab} + \frac{\boldsymbol{A}_b}{\rho_b^2} \boldsymbol{J}_b \cdot \nabla_a W_{ab} \right]$$

Arises by choice of how A is evolved.

A Better Second Derivative

- One option for the kernel second derivative is to use a higher order spline.
- (In fact, Daniel needed to use the quintic spline to achieve any progress here.)

- A second option is to use a different kernel.
- I have been testing an integral approach to derivatives (Garcia-Senz, et al, 2012).
- Define the kernel gradient as:

$$\nabla_a W_{ab} \sim \mathcal{A}_{i,ab}(h_a) = \sum_{j=1}^{d} c_{ij,a}(h_a)(x_{j,b} - x_{j,a})W_{ab}(h_a)$$

$$C = \mathcal{T}^{-1}$$

$$\tau_{ij,a} = \sum_b \frac{m_b}{\rho_b}(x_{i,b} - x_{i,a})(x_{j,b} - x_{j,a})W_{ab}(h_a)$$

A Better Second Derivative

- This may just avoid a direct second derivative of the kernel!
- Might very well solve the second term of the force equation!

- But may (and probably likely) introduce more complication without providing a solution. Time will tell.

Summary

Summary

- **Modern SPMHD is robust and widely applicable.**
- Has been used to study a wide range of astrophysical problems.
- Resistive MHD can be included (Ohmic, Ambipolar, Hall).
- All of this is in Phantom!

- The foolish quest to find a truly divergence-free SPMHD continues.
- A solution remains elusive, but this is ok because standard SPMHD works well for almost all problems.
- There is some slight glimmer of hope for progress beyond our current state.